

=> d his

(FILE 'HOME' ENTERED AT 10:48:35 ON 21 DEC 2006)

FILE 'CASREACT' ENTERED AT 10:48:46 ON 21 DEC 2006

L1 STRUCTURE UPLOADED
L2 26 S L1
L3 521 S L1 FULL
L4 69 S L3 AND COPPER

=> => d his

(FILE 'HOME' ENTERED AT 10:48:35 ON 21 DEC 2006)

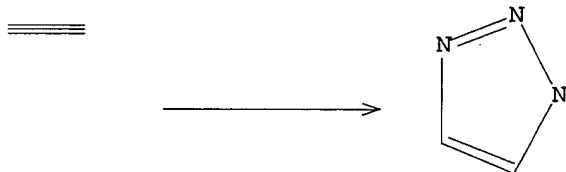
FILE 'CASREACT' ENTERED AT 10:48:46 ON 21 DEC 2006

L1 STRUCTURE UPLOADED
L2 26 S L1
L3 521 S L1 FULL
L4 69 S L3 AND COPPER

FILE 'CASREACT' ENTERED AT 10:53:48 ON 21 DEC 2006

=> d que l4 stat

L1 STR



N.....N.....N

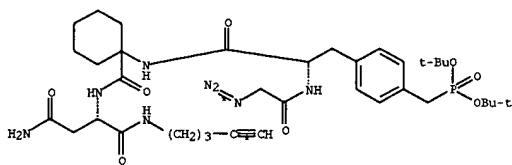
Structure attributes must be viewed using STN Express query preparation.

L3 521 SEA FILE=CASREACT SSS FUL L1 (10377 REACTIONS)
L4 69 SEA FILE=CASREACT ABB=ON PLU=ON L3 AND COPPER

=> d 1-69 bib abs fhit

L4 ANSWER 1 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:489546 CASREACT
 TI Application of azide-alkyne cycloaddition 'click chemistry' for the synthesis of Grb2 SH2 domain-binding macrocycles
 AU Choi, Won Jun; Shi, Zhen-Dan; Worthing, Karen M.; Bindu, Lakshman; Karki, Rajeshri G.; Nicklaus, Marc C.; Fisher, Robert J.; Burke, Terrence R.
 CS Laboratory of Medicinal Chemistry, CCR, NCI, NIH, Frederick, MD, 21702, USA
 SO Bioorganic & Medicinal Chemistry Letters (2006), 16(20), 5265-5269
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Ltd.
 DT Journal
 LA English
 AB Copper(I)-promoted [3+2] Huisgen cycloaddn. of azides with terminal alkynes was used to prepare triazole-containing macrocycles based on the Grb2 SH2 domain-binding motif, Pmp-Ac6c-Azn', where Pmp and Ac6c stand for 4-phosphonomethylphenylalanine and 1-aminocyclohexanecarboxylic acid, resp. When cycloaddn. reactions were conducted at 1 mM substrate concns., cyclization of monomeric units occurred. At 2 mM substrate concns., the predominant products were macrocyclic dimers. In Grb2 SH2 domain-binding assays the monomeric (S)-Pmp-containing macrocycle exhibited a K_d value of 0.23 μM, while the corresponding dimeric macrocycle was found to have greater than 50-fold higher affinity. The open-chain dimer was also found to have affinity equal to the dimeric macrocycle. This work represents the first application of "click chemical" to the synthesis of SH2 domain-binding inhibitors and indicates its potential utility.

RX(9) OF 197 ...3 V ==> AA + AB...



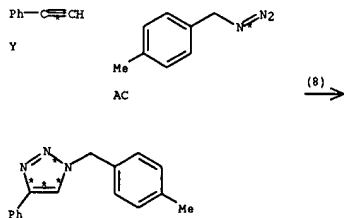
3 V

(9) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L4 ANSWER 2 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:271150 CASREACT
 TI Catalyst Recycling via Hydrogen-Bonding-Based Affinity Tags
 AU Gruijters, Bas W. T.; Broeren, Maarten A. C.; Van Delft, Floris L.; Sijbesma, Rint P.; Hermkens, Pedro H. H.; Rutjes, Floris P. J. T.
 CS Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, NL-6525 ED, Neth.
 SO Organic Letters (2006), 8(15), 3163-3166
 CODEN: ORLEP7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 AB A novel procedure for catalyst recycling is described. Copper (I)-based catalysts, equipped with an affinity tag, are isolated from crude reaction mixts. on the basis of quadruple hydrogen-bonding interactions using a resin functionalized with complementary affinity tags. Recycled catalysts were successfully used to catalyze a tandem Sonogashira coupling/5-endo-dig cyclization and a Cu-catalyzed [3+2] Huisgen cycloaddn. reaction in high yields.

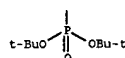
RX(8) OF 13 Y + AC ==> AD



AD
 YIELD 99%

RX(8) RCT Y 536-74-3, AC 17271-89-5
 PRO AD 126800-02-0
 CAT 25753-84-8 Copper, bromo(1,10-phenanthroline-κN1,κN10)(triphenylphosphine)-, (T-4)-
 SOL 75-05-8 MeCN
 CON 16 hours, room temperature
 NTE Huisgen reaction, in-situ generated catalyst
 RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 1 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 PAGE 2-B

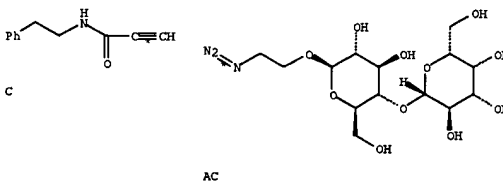


AB
 YIELD 26%

RX(9) RCT V 914459-79-3
 RGT AC 134-03-2 Na ascorbate, AD 7087-68-5 EtN(Pr-i)2
 PRO AA 914459-82-8, AB 914459-84-0
 CAT 7681-65-4 CuI
 SOL 7732-18-5 Water, 67-56-1 MeOH, 75-65-0 t-BuOH
 CON room temperature
 NTE product depends on concn.
 RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

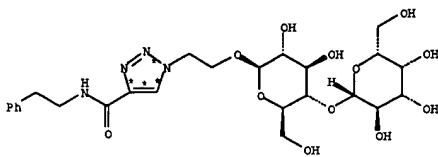
L4 ANSWER 3 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:211311 CASREACT
 TI Synthesis of multivalent lactose derivatives by 1,3-dipolar cycloadditions: selective galectin-1 inhibition
 AU Tejler, Johan; Tullberg, Erik; Frejd, Torbjørn; Leffler, Hakon; Nilsson, Ulf J.
 CS Organic Chemistry, Lund University, Lund, SE-221 00, Swed.
 SO Carbohydrate Research (2006), 341(10), 1353-1362
 CODEN: CRBRAT; ISSN: 0008-6215
 PB Elsevier B.V.
 DT Journal
 LA English
 AB Acetylene derivs. of phenylalanine, phenethylamine and the multifunctional unnatural amino acids, phenyl-bis-alanine and phenyl-tris-alanine, were synthesized and functionalized with 2-azidoethyl β--galactopyranosyl-(1-4)-β-D-glucopyranoside via regioselective copper (I)-mediated 1,3-dipolar cycloaddn. to give a panel of mono-, di- and trivalent lactoside derivs. Evaluation of the compds. as inhibitors against the tumor- and inflammation-related galectin-1, -3, -4N, -4C, -4, -7, -8N and -9N revealed a divalent compound with a K_d value as low as 3.2 μM for galectin-1, which corresponded to a relative potency of 30 per lactose unit as compared to the natural disaccharide ligand lactose. This divalent compound had at least one order of magnitude higher affinity for galectin-1 than for any of the other galectins investigated.

RX(11) OF 32 ...C + AC ==> AD



(11) →

L4 ANSWER 3 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

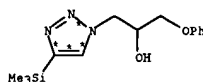
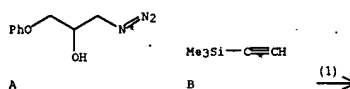
AD
YIELD 66%

RX(11) RCT C 146722-56-7, AC 230286-11-0
 RGT AE 7087-68-5 EtN(Pr-1)2
 PRO AD 904704-11-6
 CAT 7681-65-4 CuI
 SOL 75-05-8 MeCN
 CON 6 days, room temperature
 RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 145:188805 CASREACT
 TI Synthesis of 1,4,5-trisubstituted-1,2,3-triazoles by copper
 -catalyzed cycloaddition-coupling of azides and terminal alkynes
 AU Gerard, Baudouin; Ryan, Jamie; Seiler, Aaron B.; Porco, John A., Jr.
 CS Department of Chemistry, Center for Methodology and Library Development,
 Boston University, Boston, MA, 02215, USA
 SO Tetrahedron (2006), 62(26), 6405-6411
 CODEN: TETRA; ISSN: 0040-4020
 PB Elsevier B.V.
 DT Journal
 LA English
 AB Primary, secondary, and aromatic azides undergo 1,3 dipolar
 cycloaddn.-coupling with an excess of alkyne in the presence of
 Cu(MeCN)4PF6 as catalyst, N,N,N',N'-trimethylethylenediamine as ligand, mol.
 oxygen, and 4-methoxymorpholine N-oxide (NMO) as co-oxidant to afford
 1,4,5-trisubstituted-1,2,3-triazoles.

RX(1) OF 14 A + B ==> C

C
YIELD 48%

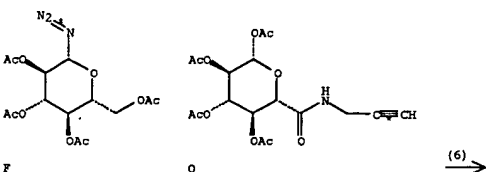
RX(1) RCT A 121282-65-3, B 1066-54-2
 PRO C 902489-55-8
 CAT 7087-68-5 EtN(Pr-1)2, 7681-65-4 CuI
 SOL 109-99-9 THF
 CON SUBSTAGE(1) 30 minutes, room temperature
 SUBSTAGE(2) 12 hours, room temperature
 RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:167475 CASREACT
 TI N-Glycoside neoglycotrimers from 2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl azide
 AU Temelkoff, David P.; Zeller, Matthias; Norris, Peter
 CS Department of Chemistry, Youngstown State University, Youngstown, OH,
 44555-3663, USA
 SO Carbohydrate Research (2006), 341(9), 1081-1090
 CODEN: CARB; ISSN: 0008-6215
 PB Elsevier B.V.
 DT Journal
 LA English
 GI

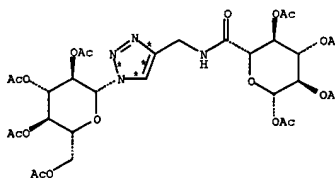
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 2,3,4,6-Tetra-O-acetyl-β-D-glucopyranosyl azide is available on large
 scale from D-glucose by means of a three-step sequence involving
 acetylation, activation as the glycosyl bromide, and stereospecific
 displacement with azide anion. The azide functionality then serves as a
 convenient anchor upon which to introduce new functionality, usually with
 retention of the β-stereochem. The synthesis of two types of
 amide-linked neoglycotrimers is reported. An amide-linked trimer I was
 prepared via Staudinger-aza-Wittig chemical using
 bis(diphenylphosphino)ethane
 (dippe) as the phosphine to avoid the workup problems associated with other
 phosphines. A triazole-linked trimer II was prepared via regioselective
 Cu(I)-catalyzed dipolar cycloaddn. between glycosyl azides and a
 glucopyranuronosyl-derived alkyne with retention of stereochem. at each
 anomeric center. Both of these neoglycotrimers were isolated in good
 yield with high β-selectivity in each case.

RX(6) OF 34 ...F + Q ==> T...



L4 ANSWER 5 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

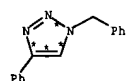
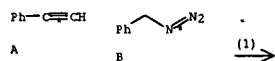
T
YIELD 91%

RX(6) RCT F 13992-25-1, Q 900177-12-0
 STAGE(1)
 RGT U 7758-98-7 CuSO4, V 62624-30-0 Ascorbic acid
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 60 deg C
 SUBSTAGE(2) 60 deg C -> room temperature
 STAGE(2)
 SOL 7732-18-5 Water
 CON room temperature

PRO T 900177-13-1
 RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:167169 CASREACT
 TI Copper(II)-promoted regioselective synthesis of
 1,4-disubstituted 1,2,3-triazoles in water
 AU Reddy, K. Rajender; Rajgopal, K.; Kantam, M. Lakshmi
 CS Inorganic and Physical Chemistry Division, Indian Institute of Chemical
 Technology, Hyderabad, 500007, India
 SO Synlett (2006), (6), 957-959
 CODEN: SYNLES; ISSN: 0936-5214
 PB Georg Thieme Verlag
 DT Journal
 LA English
 AB A high-yielding synthesis of 1,2,3-triazole with cheaply available
 Cu(OAc)₂ without any addnl. reducing agents is explored, which provides an
 exclusive 1,4-regioselectivity at ambient conditions in an environmentally
 benign solvent - water.

RX(1) OF 7 A + B ==> C

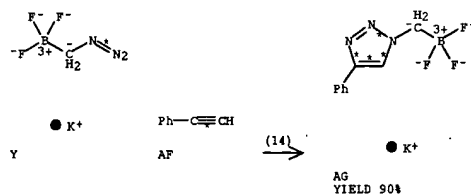


YIELD 100%

RX(1) RCT A 536-74-3, B 622-79-7
 PRO C 108717-96-0
 CAT 7681-65-4 CuI
 SOL 7732-18-5 Water
 CON 20 hours, room temperature
 NTE green chemistry-solvent, regioselective
 RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

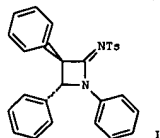
L4 ANSWER 7 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:145777 CASREACT
 TI Synthesis of Functionalized Organotrifluoroborates via the 1,3-Dipolar
 Cycloaddition of Azides
 AU Molander, Gary A.; Ham, Jungyeob
 CS Roy and Diana Vagelos Laboratories, Department of Chemistry, University of
 Pennsylvania, Philadelphia, PA, 19104-6323, USA
 SO Organic Letters (2006), 8(13), 2767-2770
 CODEN: ORLEP7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 AB 1-Alkynes undergo 1,3-dipolar addition with (azidoalkyl)- and
 [(azidoalkyl)phenyl]trifluoroborates, affording triazolyl-substituted
 organotrifluoroborates in one-pot copper-catalyzed reaction
 starting from haloalkyl derivs. Reaction of RC.tpbond.CH with
 [N3CH2BF3]K gave [4-RC2HN3-1-CH2BF3]K [12-16; R = Ph, CH2OH, Eto2C,
 cyclohexylmethyl, Bu, NC(CH2)3, PhSCH2, 1-naphthyl, PhCH2CH2CH2] with
 85-98% yields. One-pot reaction of [XQBF3]K [X = Cl, Br; Q = (CH2)5,
 2-C6H4CH2, 3-C6H4CH2, 4-C6H4CH2] with NaN3 and PhC.tpbond.CH or
 Eto2CC.tpbond.CH gave the corresponding triazolyl borates
 [4-RC2HN3-1-QBF3]K with 92-97% yields.

RX(14) OF 103 ...Y + AF ==> AG



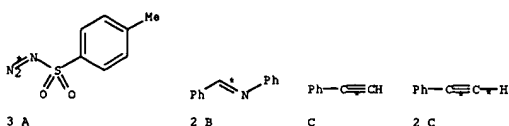
RX(14) RCT Y 898544-47-3, AF 536-74-3
 PRO AG 898544-51-9
 CAT 7681-65-4 CuI
 SOL 2206-27-1 DMSO-d6
 CON SUBSTAGE(1) room temperature -> 80 deg C
 SUBSTAGE(2) 1 hour, 80 deg C
 NTE optimization study, regioselective
 RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:145471 CASREACT
 TI Copper-catalyzed reaction cascade: direct conversion of alkynes
 into N-sulfonylazetidin-2-imines
 AU Whiting, Matthew; Fokin, Valery V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
 92037, USA
 SO Angewandte Chemie, International Edition (2006), 45(19), 3157-3161
 CODEN: AClEFS; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 GI

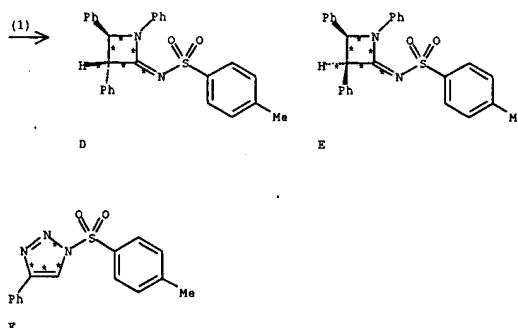


AB Densely functionalized azetidine derivs. are formed in an exptl. simple
 three-component catalytic procedure through the highly selective reaction
 of readily available terminal alkynes under mild conditions. Thus,
 reaction of TsN₃, PhC.tpbond.CH, and PhN:CHPh in presence of CuI/pyridine
 gave N-sulfonylazetidin-2-imine I (90% yield, >95:5 trans:cis). The
 azetidine products are remarkably stable to a wide range of reaction
 conditions and readily undergo further functionalization.

RX(1) OF 41 3 A + 2 B + 3 C ==> D + E +



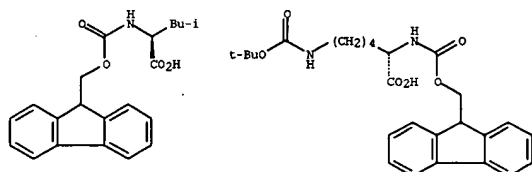
L4 ANSWER 8 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 941-55-9, B 538-51-2, C 536-74-3
 PRO D 898911-89-2, E 898911-90-5, F 898911-90-5
 CAT 7681-65-4 CuI, 108-48-5 2,6-Lutidine
 SOL 75-05-8 MeCN
 CON 3 hours, room temperature
 NTE trans-4 member ring:cis-4 member ring: 5-member ring 80:13:7,
 stereoselective
 RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 145:124835 CASREACT
 TI Synthesis of 2-alkoxy-8-hydroxyadenylpeptides: Towards synthetic
 epitope-based vaccines
 AU Weterings, Jimmy J.; Khan, Selina; Van der Heden, Gerbrand J.; Drijfhout,
 Jan W.; Melief, Cornelis J. M.; Overkleeft, Herman S.; Van der Burg,
 Sjoerd H.; Ossendorp, Ferry; Van der Marel, Gijbert A.; Filippov, Dmitri
 V.
 CS Leiden Institute of Chemistry, Leiden University, Leiden, 2300 RA, Neth.
 SO Bioorganic & Medicinal Chemistry Letters (2006), 16(12), 3258-3261
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier B.V.
 DT Journal
 LA English
 AB The preparation of three different 2-alkoxy-8-hydroxyadenylpeptide
 conjugates
 has been accomplished by solid-phase synthesis combined with 'on-resin'
 Cu(I) catalyzed Huisgen cycloaddn. of azide to alkyne. The immunogenicity
 of the compds. has been evaluated in IL-12 production and antigen
 presentation assays.

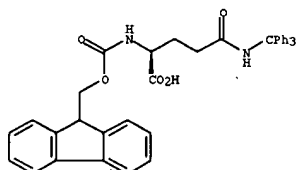
RX(6) OF 33 ... 2 T + U + V + W + X + Y + Z + AA + AB + AC
 + AD + AE + Q ==> AF



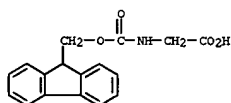
2 T

U

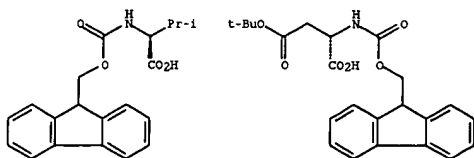
L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AA

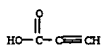


AB



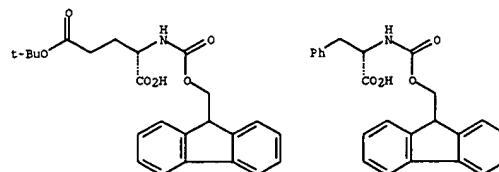
AC

AD



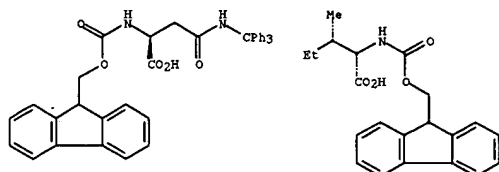
AE

L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



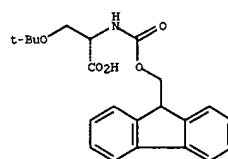
V

W



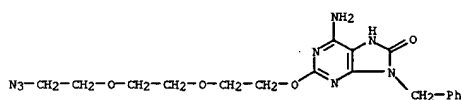
X

Y



Z

L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



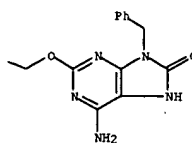
Q

(6)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 1-C



||
O

PAGE 2-A

AF
YIELD 41

RX(6) RCT T 35661-60-0

STAGE(1)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMMP
CON 15 minutes, room temperature

STAGE(2)
RCT U 71989-26-9
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-1)2
SOL 872-50-4 NMMP
CON 45 minutes, room temperature

L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(3)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(4)
RCT V 71989-18-9
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(5)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(6)
RCT W 35661-40-6
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(7)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(8)
RCT X 132388-59-1
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(9)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(10)
RCT Y 71989-23-6
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(11)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(12)
RCT Z 71989-33-8
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(13)

L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

CON 15 minutes, room temperature

STAGE(24)
RCT AE 471-25-0
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 2 hours, room temperature

STAGE(25)
RCT Q 897050-09-8
RGT AI 7087-68-5 EtN(Pr-i)2
CAT 7681-65-4 CuI
SOL 872-50-4 NMEP
CON 48 hours, room temperature

STAGE(26)
RGT AJ 6485-79-6 Silane, tris(1-methylethyl)-, S 7732-18-5
Water, AK 76-05-1 F3CCO2H
CON 2 hours, room temperature

PRO AF 897050-10-1
NTE automated peptide synthesizer and Fmoc based protocol used from Fmoc-Leu-PHB-Tentagel resin, stage 25 chemoselective Huisgen cycloaddition, acetic anhydride capping steps omitted, solid-supported reaction

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(14)
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(15)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(16)
RCT AA 132327-80-1
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(17)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(18)
RCT AB 29022-11-5
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(19)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(20)
RCT AC 68858-20-8
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(21)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP
CON 15 minutes, room temperature

STAGE(22)
RCT AD 71989-14-5
RGT AH 490019-20-0, AI 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP
CON 45 minutes, room temperature

STAGE(23)
RGT AG 110-89-4 Piperidine
SOL 872-50-4 NMEP

L4 ANSWER 10 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 14546043 CASREACT

TI Macrocyclizations Leading to Conformationally Restricted Small Molecules

AU Loofer, Ryan E.; Pizzirani, Daniela; Schreiber, Stuart L.

CS Howard Hughes Medical Institute, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SO Organic Letters (2006), 8(10), 2063-2066

CODEN: ORLEF7; ISSN: 1523-7060

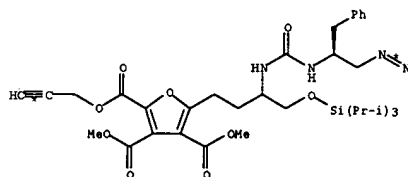
PB American Chemical Society

DT Journal

LA English

AB The Cu(I)-catalyzed cycloaddn. of alkynes and azides (click reaction) provides a robust method for the construction of macrocyclic small mols. via intramol. macrocycloaddn. Diazodicarbonylpropylpyrrolidines are prepared in one step from nonracemic (triisopropylsilyloxymethyl)pyrrolidinone 5; a one-pot three-component coupling reaction consisting of rhodium-catalyzed cycloaddn. with di-Me acetylenedicarboxylate, retro-Diels-Alder cycloaddn., and amine addition to the in-situ-generated isocyanates leads to nonracemic acyclic ureas which can be further functionalized. Copper-catalyzed regioselective cycloaddn. of azides and alkynes yields the product macrocycles with small amts. of intermol. cycloaddn. products. Variation of the starting materials allows access to macrocycloaddn. precursors with differing stereochemistries and substituents for exploration of the tolerance of azide-alkyne macrocycloaddn. to structural and stereochem. variations.

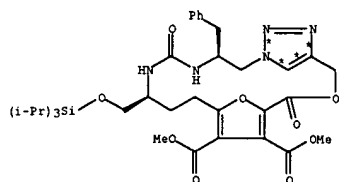
RX(39) OF 247 ...U ==> BR...



U

(39) →

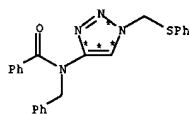
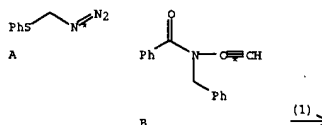
L4 ANSWER 10 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

BR
YIELD 67%

RX(39) RCT U 890139-50-1
 RGT AV 7087-68-5 EtN(Pr-1)2, BS 7681-65-4 CuI
 PRO BR 890139-94-3
 SOL 108-88-3 PhMe
 CON 12 hours, room temperature
 RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:488891 CASREACT
 TI Click chemistry with ynamides
 AU IJssels, Maarten; Cintrat, Jean-Christophe
 CS DSV/DSJC/Service de Marquage Moléculaire et de Chimie Bioorganique, CEA/Saclay, Gif sur Yvette, 91191, Fr.
 SO Tetrahedron (2006), 62(16), 3837-3842
 CODEN: TETRAH; ISSN: 0040-4020
 PB Elsevier B.V.
 DT Journal
 LA English
 AB A series of diversely 1-substituted 4-amino 1,2,3-triazoles were synthesized by [3+2] cycloaddn. between azides and ynamides. This copper catalyzed process represents the first examples of a click reaction' employing ynamides and should expand the scope of the ynamide chemical both synthetically and industrially. Various azides (even highly functionalized) were allowed to react with N-benzyl, N-tosyl ynamide to give the corresponding triazole adducts in high yield and with very high levels of regioselectivity.

RX(1) OF 11 A + B ==> C

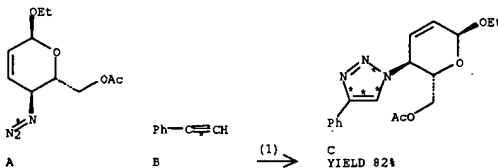
C
YIELD 55%

RX(1) RCT A 77422-70-9, B 205885-41-2
 RGT D 134-03-2 Na ascorbate
 PRO C 887402-64-4
 CAT 142-71-2 Cu(OAc)2
 SOL 7732-18-5 Water, 75-65-0 t-BuOH, 67-66-3 CHCl3
 CON overnight, room temperature
 NTE regioselective

L4 ANSWER 11 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:488858 CASREACT
 TI A very simple synthesis of 1-(ethyl 6-O-acetyl-2,3,4-trideoxy-α-D-erythro-hex-2-enopyranos-4-yl)-1,2,3-triazole derivatives
 AU de Oliveira, Ronaldo N.; Sinou, Denis; Srivastava, Rajendra M.
 CS Laboratoire de Synthèse Asymétrique, UMR 5181, ESCPE Lyon, Université Claude Bernard Lyon 1, Villeurbanne, 69662, Fr.
 SO Synthesis (2006), (3), 467-470
 CODEN: SYNTHS; ISSN: 0039-7881
 PB Georg Thieme Verlag
 DT Journal
 LA English
 AB The copper-catalyzed reaction of Et 4-azido-6-O-acetoxy-2,3,4-trideoxy-α-D-erythro-hex-2-enopyranoside with various functionalized alkynes gave the corresponding 1-(Et 6-O-acetyl-2,3,4-trideoxy-α-D-erythro-hex-2-enopyranos-4-yl)-1,2,3-triazole derivs. in quite good yields, which could be transformed into (Et 2,3,6-tri-O-acetyl-4-deoxy-α-D-mannopyranosyl)-1H-1,2,3-triazole by a simple bis-hydroxylation.

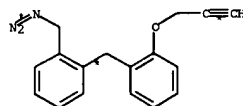
RX(1) OF 9 A + B ==> C



RX(1) RCT A 864851-94-5, B 536-74-3
 RGT D 134-03-2 Na ascorbate
 PRO C 887340-60-5
 CAT 142-71-2 Cu(OAc)2
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON overnight, room temperature
 RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

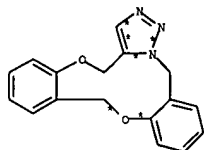
L4 ANSWER 13 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:468381 CASREACT
 TI Cu(I)-Catalyzed cycloaddition of constrained azido-alkynes: access to 12- to 17-membered monomeric triazolophanes incorporating furanoside rings
 AU Ray, Ankur; Manoj, K.; Bhadbhade, Mohan M.; Mukhopadhyay, Ranjan; Bhattacharjya, Anup
 CS Chemistry Division, Indian Institute of Chemical Biology, Kolkata, West Bengal, 700032, India
 SO Tetrahedron Letters (2006), 47(16), 2775-2778
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier B.V.
 DT Journal
 LA English
 AB A strained monomeric 12-membered triazolophane was formed by the Cu(I)-catalyzed intramol. cycloaddn. of an azide to an alkyne having a constrained tether incorporating an aromatic ring and a furanoside ring. Similar cycloaddns. of azido-alkynes having ester, furanoside and peptidic tethers led to the formation of monomeric triazolophanes of higher ring sizes.

RX(15) OF 86 ...R ==> AK



R

(15)



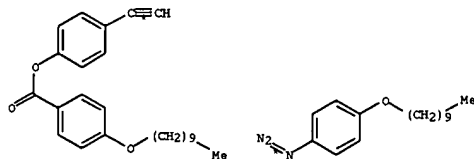
AK
 YIELD 31%

RX(15) RCT R 886969-04-6
 RGT AL 134-03-2 Na ascorbate
 PRO AK 886969-13-7
 CAT 7758-98-7 CuSO4

L4 ANSWER 13 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 12 - 24 hours, 25 deg C
 RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:379497 CASREACT
 TI New 1,4-diaryl [1,2,3]triazole liquid crystals using a click reaction
 AU Conte, Gilmar; Cristiano, Rodrigo; Ely, Fernando; Gallardo, Hugo
 CS Departamento de Química, Universidade Federal de Santa Catarina, Campus Trindade, Florianópolis, CEP 88040 900, Brazil
 SO Synthetic Communications (2006), 36(7), 951-958
 CODEN: SYNCAV; ISSN: 0039-7911
 PB Taylor & Francis, Inc.
 DT Journal
 LA English
 AB New nonlinear compds. containing 1,4-diaryl-[1,2,3]-triazole were prepared using a straightforward and efficient method for the regioselective synthesis of [1,2,3]-triazoles. The methodol. consists of a Cu(I)-catalyzed 1,3-dipolar cycloaddn. of aryl azides to terminal arylacetylenes (click reaction). All compds. exhibited liquid-crystalline profile.

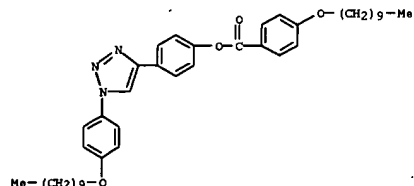
RX(2) OF 11 ...G + B ==> H



G

B

(2)



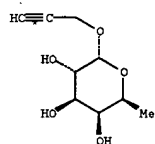
H
 YIELD 56%

RX(2) RCT G 142663-59-0
 STAGE(1)
 RGT I 121-44-8 Et3N

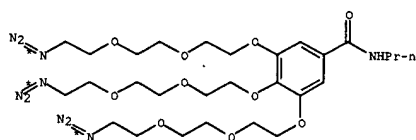
L4 ANSWER 14 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 CAT 7681-65-4 CuI
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 30 minutes, room temperature
 STAGE(2)
 RCT B 869061-55-2
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 48 hours, 60 deg C
 PRO H 882166-93-0
 NTE regioselective
 RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:370314 CASREACT
 TI A Click Approach to Unprotected Glycodendrimers
 AU Fernandez-Megia, Eduardo; Correa, Juan; Rodriguez-Meizoso, Irene; Riguera, Ricardo
 CS Departamento de Química Orgánica, Facultad de Química, and Unidad de RMN de Biomoléculas Asociada al CSIC, Universidad de Santiago de Compostela, Santiago de Compostela, 15782, Spain
 SO Macromolecules (2006), 39(6), 2113-2120
 CODEN: MAMOEY; ISSN: 0024-9297
 PB American Chemical Society
 DT Journal
 LA English
 AB Click chemical in combination with ultra-filtration has allowed the quick, efficient, and reliable multivalent conjugation of unprotected alkyne-derived carbohydrates to three generations of azido-terminated gallic acid-triethylene glycol dendrimers under aqueous conditions. The reported procedure allows the atom economical incorporation of up to 27 unprotected fucose, mannose, and lactose residues, in reproducible high yields (up to 92%), requiring only catalytic amounts of Cu. The completion of the conjugation process was clearly established in all cases by both ¹H NMR and MALDI-TOF MS.

RX(12) OF 140 ...3 AF + S ==> AO



3 AF

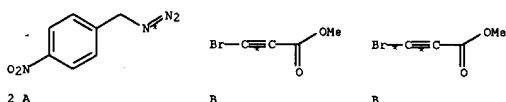


S

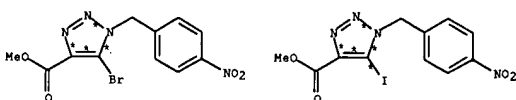
(12)

L4 ANSWER 16 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:369998 CASREACT
 TI Copper(I)-mediated synthesis of trisubstituted 1,2,3-triazoles
 AU Kuipers, Brian H. M.; Dijkman, Guido C. T.; Groothuis, Stan; Quaedflieg, Peter J. L. M.; Blaauw, Richard H.; van Delft, Floris L.; Rutjes, Floris P. J. T.
 CS Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, 6525 ED, Neth.
 SO Synlett (2005), (20), 3059-3062
 CODEN: SYNLDT; ISSN: 0936-5214
 PB Georg Thieme Verlag
 DT Journal
 LA English
 AB A copper-catalyzed coupling of bromo-alkynes and organic azides is described. This coupling results in the formation of bromo-containing trisubstituted 1,2,3-triazole derivs. in high yield and a regioselective manner.

RX(1) OF 19 2 A + 2 B ==> C + D



(1)



C
YIELD 99% (94)

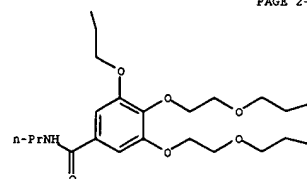
D
YIELD 99% (6)

RX(1) RCT A 17271-88-4, B 23680-40-2
 PRO C 882300-81-4, D 882300-82-5
 CAT 7681-65-4 CuI, 142-71-2 Cu(OAc)₂
 SOL 109-99-9 THF
 CON 16 hours, 50 deg C
 NTE optimized on catalysts and reaction conditions, regioselective
 RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

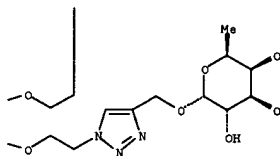
L4 ANSWER 15 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B

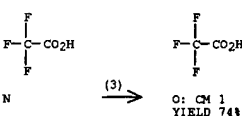
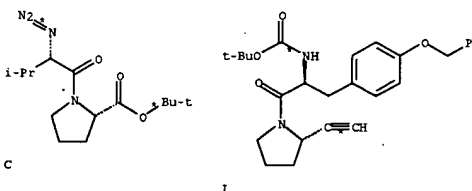


AO
YIELD 79%

RX(12) RCT AF 882168-36-7, S 882168-49-2
 RGT AP 134-03-2 Na ascorbate, AQ 7758-98-7 CuSO₄
 PRO AO 882168-52-7
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 24 hours, room temperature
 RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

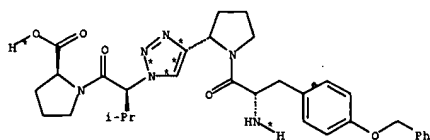
L4 ANSWER 17 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:350963 CASREACT
 TI Click chemistry as a route to cyclic tetrapeptide analogs: Synthesis of cyclo-[Pro-Val-w(triazole)-Pro-Tyr]
 AU Bock, Victoria D.; Perciaccante, Rossana; Jansen, T. Paul; Hiemstra, Henk; Van Maarseveen, Jan H.
 CS Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, 1018 WS, Neth.
 SO Organic Letters (2006), 8(5), 919-922
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 AB Despite the plethora of techniques to cyclize small peptides, a synthesis of cyclo-[LPro-(L)Tyr-(L)Pro-(L)Val], a potent tyrosinase inhibitor, remains elusive because of the unfavorable transition state leading to the cyclic product. Herein, we report the successful synthesis of its triazole analog, cyclo-[LPro-(L)Val-w(triazole)-(L)Pro-(L)Tyr]. Attempted cyclization via peptide bond formation at room temperature fails to provide the desired product, but CuI-catalyzed alkyne-azide coupling at 110° affords the triazole tetrapeptide in 70% yield, demonstrating the utility of "click" chemical

RX(3) OF 60 ...C + I + N ==> O



O: CM 1
YIELD 74%

L4 ANSWER 17 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

O: CM 2
YIELD 74%

RX(3) RCT C 881691-87-8, I 881691-88-9

STAGE(1)

RGT K 7087-68-5 EtN(Pr-1)2, P 108-48-5 2,6-Lutidine
CAT 7681-65-4 CuI
SOL 109-99-9 THF, 75-05-8 MeCN
CON 16 hours, room temperature

STAGE(2)

RGT Q 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON room temperature

STAGE(3)

RCT N 76-05-1
SOL 67-66-3 CHCl3
CON 5 hours, room temperature

PRO O 881691-85-6

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 144:292672 CASREACT

TI Efficient synthesis of 1,4-disubstituted 1,2,3-triazoles in ionic liquid/water system

AU Zhao, Ya-Bin; Yan, Ze-Yi; Liang, Yong-Min

CS State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China

SO Tetrahedron Letters (2006), 47(10), 1545-1549

CODEN: TELEAY; ISSN: 0040-4039

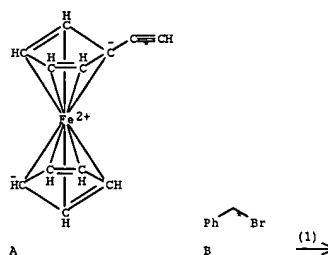
PB Elsevier B.V.

DT Journal

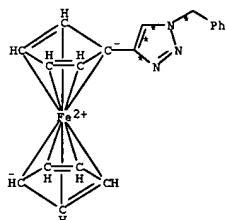
LA English

AB A copper(I) catalyst in a mixture of the ionic liquid [bmim][BF4] and water, can effect three-component reaction of halides, sodium azide, and alkynes to form 1,4-disubstituted 1,2,3-triazoles in good to high yields. The method is efficient and environmentally friendly.

RX(1) OF 16 A + B ==> C



L4 ANSWER 18 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

C
YIELD 99%

RX(1) RCT A 1271-47-2, B 100-39-0

RGT D 26628-22-8 NaN3

PRO C 878811-47-3

CAT 7681-65-4 CuI

SOL 174501-65-6 1H-Imidazolium, 1-butyl-3-methyl-,

tetrafluoroborate(1-), 7732-18-5 Water

CON 8 hours, room temperature

NTE green chem., solvent, regioselective, Huisgen cycloaddition reaction, multicomponent reaction

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 144:192189 CASREACT

TI Efficient one-pot synthesis of 1-aryl 1,2,3-triazoles from aryl halides and terminal alkynes in the presence of sodium azide

AU Andersen, Jacob; Bolvig, Simon; Liang, Xifu

CS Department of Medicinal Chemistry, LEO Pharma, Ballerup, 2750, Den.

SO Synlett (2005), (19), 2941-2947

CODEN: SYNLES; ISSN: 0936-5214

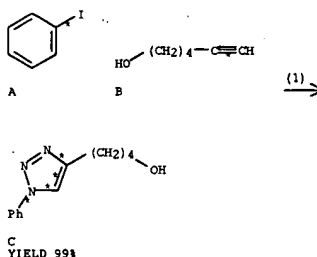
PB Georg Thieme Verlag

DT Journal

LA English

AB An efficient one-pot synthesis of 1-aryl-1,2,3-triazoles from aryl bromides/iodides and terminal alkynes in the presence of sodium azide is described. In the case of aryl iodides, the reactions proceeded at room temperature. The reactions normally gave high yields.

RX(1) OF 25 A + B ==> C

C
YIELD 99%

RX(1) RCT A 591-50-4, B 928-90-5

RGT D 26628-22-8 NaN3

PRO C 875312-68-8

CAT 7681-65-4 CuI, 67579-81-1 1,2-Cyclohexanediamine,

N,N'-dimethyl-, (1R,2R)-rel-, 134-03-2 Na ascorbate

SOL 7732-18-5 Water, 67-68-5 DMSO

CON SUBSTAGE(1) room temperature

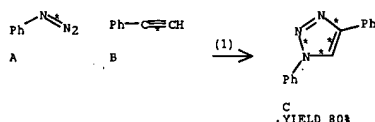
SUBSTAGE(2) 90 minutes, room temperature

NTE regioselective

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:152183 CASREACT
 TI Click chemistry: copper clusters catalyze the cycloaddition of azides with terminal alkynes
 AU Pachon, Laura Duran; van Maarseveen, Jan H.; Rothenberg, Gadi
 CS van't Hoff Inst. of Mol. Sci., Univ. of Amsterdam, Amsterdam, 1018 WV, Neth.
 SO Advanced Synthesis & Catalysis (2005), 347(6), 811-815
 CODEN: ASCAP7; ISSN: 1615-4150
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 AB Air-stable copper nanoclusters are good catalysts in the Cu(I)-catalyzed "click" cycloaddn. of azides with terminal alkynes to give 1,4-disubstituted 1,2,3-triazoles. No addnl. base or reducing agent is required. The reaction kinetics using various copper catalyst types and the function of copper particles in this system are studied and discussed.

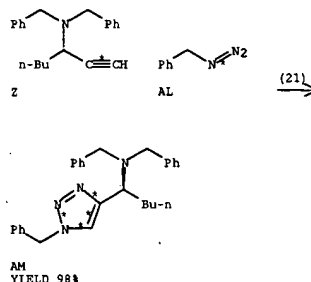
RX(1) OF 6 A + B ==> C



RX(1) RCT A 622-37-7, B 536-74-3
 PRO C 13148-78-2
 CAT 7440-50-8 Cu
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 18 hours, 25 deg C
 RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:108259 CASREACT
 TI Enantioselective synthesis of chiral α-aminoalkyl-1,2,3-triazoles using a three-component reaction
 AU Gommermann, Nina; Gehrig, Anna; Knochel, Paul
 CS Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Munich, 81377, Germany
 SO Synlett (2005), (10), 2796-2798
 CODEN: SYNLES; ISSN: 0936-5214
 PB Georg Thieme Verlag
 DT Journal
 LA English
 AB A range of chiral α-aminoalkyl-1,2,3-triazoles were prepared in a modular fashion in 3 steps with up to 98% ee. The key step is a CuBr/Quinap-catalyzed enantioselective asym. three-component synthesis of propargylamines.

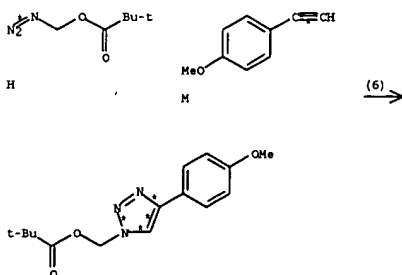
RX(21) OF 63 ...Z + AL ==> AM



RX(21) RCT Z 780782-33-4, AL 622-79-7
 PRO AM 872713-40-1
 CAT 7440-50-8 Cu
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 8 days, room temperature
 RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:107989 CASREACT
 TI NH-1,2,3-triazoles from azidomethyl pivalate and carbamates: Base-labile N-protecting groups
 AU Loren, Jon C.; Krasinski, Antoni; Fokin, Valery V.; Sharpless, K. Barry
 CS The Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Synlett (2005), (18), 2847-2850
 CODEN: SYNLES; ISSN: 0936-5214
 PB Georg Thieme Verlag
 DT Journal
 LA English
 AB Protected 1,2,3-triazoles are prepared by copper-catalyzed dipolar cycloaddn. reactions of acyloxymethyl azides RCOOCH2N3 (R = Me3C, 4-morpholinyl, Et2N) and terminal alkynes; the products are readily deprotected with aqueous sodium hydroxide followed by neutralization to yield 1,2,3-triazoles, with the ease of deprotection dependent upon the protecting group chosen. Pivaloyloxymethyl azide is prepared by reaction of chloromethyl pivalate with sodium azide, while 4-(azidomethoxycarbonyl)morpholine and diethylcarbamoyloxymethyl azide are prepared by addition of morpholine or diethylamine to chloromethyl chloroformate followed by reaction of the chloromethyl carbamates with sodium azide; the azides are easily prepared on 0.1-mol scale. The acyl groups determine the rate of deprotection of the protected triazoles; N-(pivaloyloxymethyl)triazoles are cleaved to 1,2,3-triazoles by treatment with aqueous sodium hydroxide for 30 min. at room temperature, while the corresponding (morpholinylcarbamoyloxymethyl)triazoles require 24 h at ambient temperature for cleavage, and the (diethylcarbamoyloxymethyl)triazoles require 24 h at 85° for cleavage. The acyloxymethyl azides are potential synthetic equivalent for hydrazoic acid in copper-catalyzed 1,3-dipolar cycloaddns.

RX(6) OF 186 ...H + M ==> N...

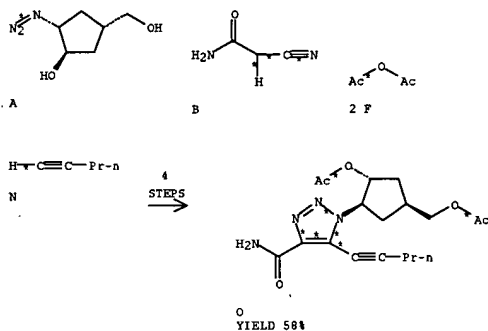


L4 ANSWER 22 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(6) RCT H 872700-68-0, M 768-60-5
 RGT O 134-03-2 Na ascorbate
 PRO N 872700-71-5
 CAT 7758-98-7 CuSO4
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 24 hours, room temperature
 NTE regioselective
 RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:88506 CASREACT
 TI Efficient Pd(0)-catalyzed synthesis of 1,2,3-triazolo-3'-deoxyribonucleosides and their analogs
 AU Joubert, Nicolas; Schinazi, Raymond P.; Agrofoglio, Luigi A.
 CS Institut de Chimie Organique et Analytique, CNRS UMR-6005, Universite d'Orleans, Orleans, 45067, Fr.
 SO Tetrahedron (2005), 61(49), 11744-11750
 CODEN: TETRAH; ISSN: 0040-4020
 PB Elsevier B.V.
 DT Journal
 LA English
 AB The racemic synthesis of hitherto unknown 5-substituted-[1,2,3]-triazolo-3'-deoxyribonucleosides and [1,2,3]-triazolo-[4,5-c]pyridin-4-one analogs is described. The key iodinated intermediate was prepared in 10 steps using a malonic synthesis. Various alkynes were introduced at the C-5 position of under optimized Pd(0)-catalyzed Sonogashira cross-coupling alkylation to yield after deprotection. The synthesis of their 8-aza-3-deazapurine analogs (13a-h) was also accomplished through the hetero-annulation of internal alkynes under aqueous dimethylamine.

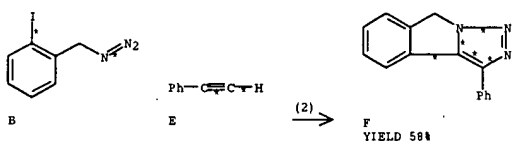
RX(68) OF 127 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
 RX(68) A + B + 2 F + N ==> O



RX(1) RCT A 872351-81-0, B 107-91-5
 RGT D 141-52-6 NaOEt
 PRO C 872351-82-1
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 20 hours, 50 deg C

L4 ANSWER 24 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:69783 CASREACT
 TI Palladium-copper catalyzed heteroannulation of acetylenic compounds: an expeditious synthesis of isoindoline fused with triazoles
 AU Chowdhury, Chinmay; Mandal, Sukhendu B.; Achari, Basudeb
 CS Process and Product Development, Central Institute of Medicinal and Aromatic Plants, Lucknow, 226015, India
 SO Tetrahedron Letters (2005), 46(49), 8531-8534
 CODEN: TETRAH; ISSN: 0040-4039
 PB Elsevier B.V.
 DT Journal
 LA English
 AB A convenient and general method for the synthesis of isoindoline fused with triazoles from 2-iodobenzyl azide and acetylenes through palladium-copper catalysis is described.

RX(2) OF 21 ...B + E ==> F



RX(2) RCT B 405198-82-5
 STAGE(1)
 RGT G 121-44-8 Et3N
 CAT 7681-65-4 CuI, 13965-03-2 PdCl2(PPh3)2
 SOL 68-12-2 DMF
 CON 1 hour, room temperature
 STAGE(2)
 RCT E 536-74-3
 CON SUBSTAGE(1) 12 hours, room temperature
 SUBSTAGE(2) room temperature -> 115 deg C
 SUBSTAGE(3) 10 hours, 115 deg C

PRO F 871915-18-3
 RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 69 CASREACT COPYRIGHT 2006 ACS on STN* (Continued)

RX(2) RCT C 872351-82-1, F 108-24-7

STAGE(1)
 SOL 110-86-1 Pyridine
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 48 hours, room temperature

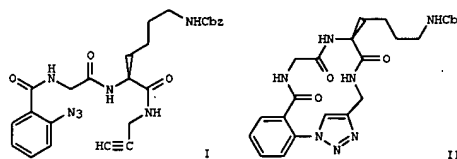
STAGE(2)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 4 hours, room temperature

PRO G 872351-83-2

RX(3) RCT G 872351-83-2
 RGT K 110-46-3 Isoamyl nitrite, L 75-11-6 CH2I2
 PRO J 872352-10-8
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 2 hours, 100 deg C
 SUBSTAGE(3) 100 deg C -> room temperature

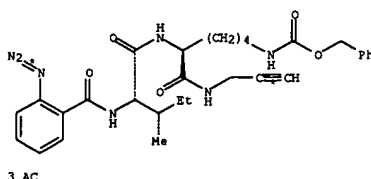
RX(4) RCT J 872352-10-8, N 627-19-0
 RGT P 121-44-8 Et3N
 PRO O 872351-84-3
 CAT 14220-64-5 PdCl2(PhCN)2
 SOL 68-12-2 DMF
 CON 4 hours, 155 deg C
 NTE yield depends on time and amt. of reactant
 RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:51877 CASREACT
 TI Ring Closure to β -Turn Mimics via Copper-Catalyzed Azide/Alkyne Cycloadditions
 AU Angell, Yu; Burgess, Kevin
 CS Chemistry Department, Texas A + M University, College Station, TX, 77842, USA
 SO Journal of Organic Chemistry (2005), 70(23), 9595-9598
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 GI

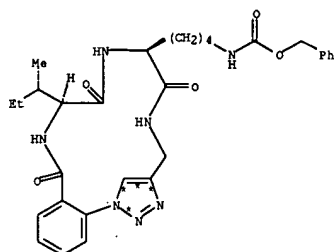


AB Copper-catalyzed azide alkyne cycloaddns. of the linear substrates were used to form the macrocyclic derivs. For example, azido-alkyne peptide I was cyclized to form macrocycle II in 14% yield. Computational, NMR, and CD analyses of these compds. indicate that their most favorable conformational states include type I and type II β -turn conformations. Selectivity for the dimeric products in these cyclization reactions is discussed.

RX(20) OF 129 ...3 AC ==> AN + AO...



L4 ANSWER 25 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AN
YIELD 12% (39)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(20) RCT AC 871117-27-0
 RGT AP 7087-68-5 EtN(Pr-i)2
 PRO AN 871117-35-0, AO 871117-43-0
 CAT 7681-65-4 CuI
 SOL 109-99-9 THF
 CON SUBSTAGE(1) 10 hours, room temperature
 SUBSTAGE(2) 4 hours, room temperature

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 144:23073 CASREACT
 TI Synthesis of a C3-symmetric (1+6)-N-acetyl-β-D-glucosamine octadeca-saccharide using click chemistry
 AU Chen, Qi; Yang, Feng; Du, Yuguo
 CS The State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, 100085, Peop. Rep. China
 SO Carbohydrate Research (2005), 340(16), 2476-2482
 CODEN: CCRBAT; ISSN: 0008-6215
 FB Elsevier B.V.
 DT Journal
 LA English
 AB A C3-sym. (1+6)-N-acetyl-β-D-glucosamine octadeca-saccharide was synthesized on the basis of a copper(I)-catalyzed 1,3-dipolar cycloaddn. reaction of azide and alkyne. The target octadeca-saccharide showed good antitumor activity against H22 in the preliminary mice tests.

RX(9) OF 79 ...Q + T ==> X...

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

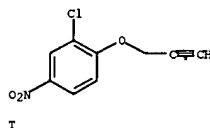
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-A



PAGE 3-B

Q



T



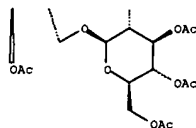
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L4 ANSWER 26 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 3-B

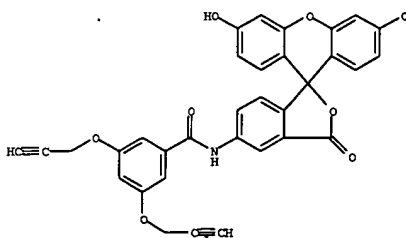
X
YIELD 60%

RX(9) RCT Q 870272-53-0, T 33126-70-4
 RGT Y 134-03-2 Na ascorbate, Z 7758-98-7 CuSO4
 PRO X 870272-54-1
 SOL 7732-18-5 Water, 109-99-9 THF
 CON 50 - 60 deg C

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

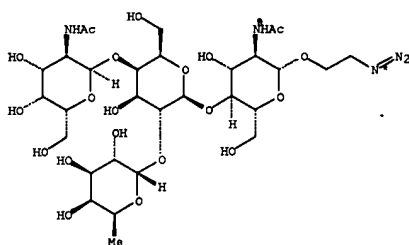
L4 ANSWER 27 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:455386 CASREACT
 TI Accelerated Bioorthogonal Conjugation: A Practical Method for the Ligation of Diverse Functional Molecules to a Polyvalent Virus Scaffold
 AU Sen Gupta, Sayam; Kuzelka, Jane; Singh, Pratik; Lewis, Warren G.; Manchester, Marianne; Finn, M. G.
 CS Department of Chemistry and the Skaggs Institute for Chemical Biology, and Department of Cell Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Bioconjugate Chemistry (2005), 16(6), 1572-1579
 CODEN: BCCHES; ISSN: 1043-1802
 FB American Chemical Society
 DT Journal
 LA English
 AB Covalent bond formation to proteins is made difficult by their multiple unprotected functional groups and normally low concns. A water-soluble sulfonated bathophenanthroline ligand (I) was used to promote a highly efficient CuI-mediated azide-alkyne cycloaddn. (CuAAC) reaction for the chemoselective attachment of biol. relevant mols. to cowpea mosaic virus (CPMV). The ligated substrates included complex sugars, peptides, poly(ethylene oxide) polymers, and the iron carrier protein transferrin, with routine success even for cases that were previously resistant to azide-alkyne coupling using the conventional ligand tris(triazolyl)amine. The use of 4-6 equiv of substrate was sufficient to achieve loadings of 60-115 mols./virion in yields of 60-85%. Although it is sensitive to oxygen, the reliably efficient performance of the Cu-I system makes it a useful tool for demanding bioconjugation applications.

RX(1) OF 7 ...A + B ==> C



A

L4 ANSWER 27 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

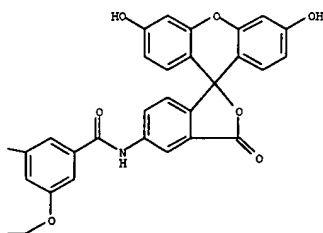


B

(1) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 1-B

C
YIELD 65%

RX(1) RCT A 869331-83-9, B 895158-74-4
 RGT D 134-03-2 Na ascorbate, E 7758-98-7 CuSO4
 PRO C 869331-81-7
 SOL 7732-18-5 Water, 75-65-0 t-BuOH, 109-99-9 THF
 CON 48 hours, room temperature
 RE.CNT 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 28 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 143:452160 CASREACT

TI Substrate activity screening: a fragment-based method for the rapid identification of nonpeptidic protease inhibitors

AU Wood, Warren J. L.; Patterson, Andrew W.; Tsuruoka, Hiroyuki; Jain, Rishi K.; Ellman, Jonathan A.

CS Department of Chemistry, University of California-Berkeley, Berkeley, CA, 94720, USA

SO Journal of the American Chemical Society (2005), 127(44), 15521-15527

CODEN: JACSAT; ISSN: 0002-7863

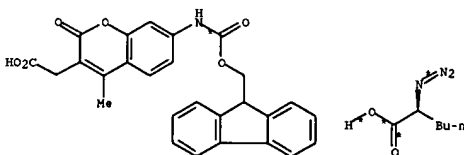
PB American Chemical Society

DT Journal

LA English

AB A new fragment-based method for the rapid development of novel and distinct classes of nonpeptidic protease inhibitors. Substrate Activity Screening (SAS), is described. This method consists of three steps: (1) a library of N-acyl aminocoumarins with diverse, low mol. weight N-acyl groups is screened to identify protease substrates using a simple fluorescence-based assay, (2) the identified N-acyl aminocoumarin substrates are optimized by rapid analog synthesis and evaluation, and (3) the optimized substrates are converted to inhibitors by direct replacement of the aminocoumarin with known mechanism-based pharmacophores. The SAS method was successfully applied to the cysteine protease cathepsin S, which is implicated in autoimmune diseases. Multiple distinct classes of nonpeptidic substrates were identified upon screening an N-acyl aminocoumarin library. Two of the nonpeptidic substrate classes were optimized to substrates with >8000-fold improvements in cleavage efficiency for each class. Select nonpeptidic substrates were then directly converted to low mol. weight, novel aldehyde inhibitors with nanomolar affinity to cathepsin S. This study demonstrates the unique characteristics and merits of this first substrate-based method for the rapid identification and optimization of weak fragments and provides the framework for the development of completely nonpeptidic inhibitors to many different proteases.

RX(1) OF 236 A + B + C ==> D



A

B

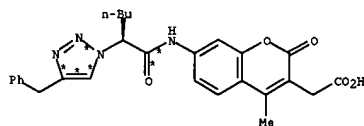
Ph-CH=CH-

C

(1) →

L4 ANSWER 27 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 28 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



D

RX(1) RCT A 884844-33-1

STAGE(1)

RGT E 4659-45-4 2,6-Cl2C6H3COC1, F 110-86-1 Pyridine

SOL 68-12-2 DMF

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 48 hours, room temperature

STAGE(2)

RGT G 110-89-4 Piperidine

SOL 68-12-2 DMF

CON 5 minutes, room temperature

STAGE(3)

RCT B 279676-22-1

RGT H 108-75-8 s-Collidine, I 148893-10-1 1H-1,2,3-Triazolo[4,5-b]pyridinium, 1-[bis(dimethylamino)methylene]-, hexafluorophosphate(1-), 3-oxide

SOL 68-12-2 DMF

CON 12 hours, room temperature

STAGE(4)

RCT C 10147-11-2

RGT J 7087-68-5 EtN(Pr-i)2

CAT 7681-65-4 CuI

SOL 109-99-9 THF

CON 20 - 48 hours, room temperature

STAGE(5)

RGT K 6485-79-6 Silane, tris(1-methylethyl)-, L 76-05-1 F3CCO2H

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 1 - 2 hour, room temperature

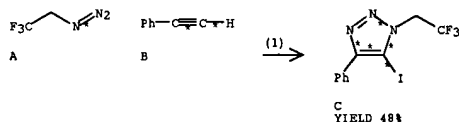
PRO D 884844-59-1

NTE combinatorial, solid-supported reaction(first stage attachment to Wang resin), other analogs similarly prepared

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:440415 CASREACT
 TI One-pot regioselective synthesis of 5-iodo-1,4-disubstituted-1,2,3-triazoles
 IN Wu, Yongming; Deng, Juan; Li, Yai Chen, Qingyun
 PA Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China
 SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 11 pp.
 CODEN: CNXKEV
 DT Patent
 LA Chinese
 FAN.CNT 1
 PATENT NO. KIND DATE APPLICATION NO. DATE
 PI CN 1583730 A 20050223 CN 2004-10024929 20040604
 PRAI CN 2004-10024929 20040604
 OS MARPAT 143:440415
 AB The invention relates to an one-pot regioselective synthesis of 5-iodo-1,4-disubstituted-1,2,3-triazole. The synthesis is achieved by carrying out reaction of organic azides, terminal alkyne, cuprous iodide, iodine monochloride, and tertiary amine in organic solvent at 10-100°C to regioselectively introduce an iodine atom onto position 5. Thus, reaction of CF₃CH₂N₃ with PhC≡Ctbbond.CH in solvent THF or MeCN in the presence of tertiary amine Bu₃N or Et₃N, CuI, and ICl at room temperature for 20 h gave 48% 5-iodo-4-phenyl-1-(2,2,2-trifluoroethyl)-1H-1,2,3-triazole.

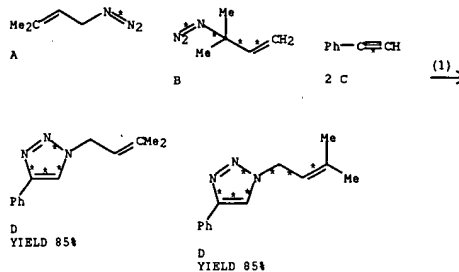
RX(1) OF 14 A + B ==> C



RX(1) RCT A 846057-92-9, B 536-74-3
 RGT D 102-82-9 Bu₃N, E 121-44-8 Et₃N, F 7790-99-0 ICl
 PRO C 860002-56-8
 CAT 7681-65-4 CuI
 SOL 109-99-9 THF, 75-05-8 MeCN, 7727-37-9 N₂
 CON 20 hours, room temperature
 NTE regioselective, either amine, either solvent

L4 ANSWER 30 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:440343 CASREACT
 TI The Allylic Azide Rearrangement: Achieving Selectivity
 AU Feldman, Aline K.; Colasson, Benoit; Sharpless, K. Barry; Fokin, Valery V.
 CS Department of Chemistry and The Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Journal of the American Chemical Society (2005), 127(39), 13444-13445
 CODEN: JACSAT; ISSN: 0002-7863
 FB American Chemical Society
 DT Journal
 LA English
 AB Allylic azides undergo a rapid [3,3]-sigmatropic rearrangement which results in dynamic equilibrium of several isomers. Thus, reactions of allylic azides usually result in mixts. of products. However, even small differences in reactivity of the isomeric allylic azides can be amplified to result in a single product in good to excellent yields. For example, the Cu(I)-catalyzed cycloaddn. with alkynes selectively captures primary and secondary allylic azide isomers, whereas MCPBA epoxidn. favors isomers which contain more electron-rich double olefins.

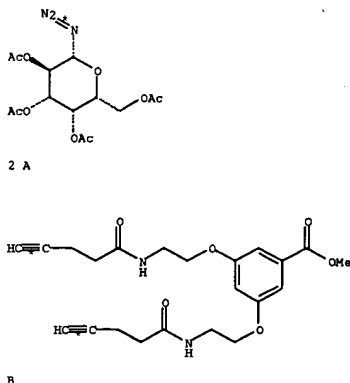
RX(1) OF 12 A + B + 2 C ==> 2 D



RX(1) RCT A 72422-42-5, B 84466-88-6, C 536-74-3
 PRO D 868684-33-7
 CAT 7758-98-7 CuSO₄, 134-03-2 Na ascorbate
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 12 hours, 23 deg C
 NTE regioselective
 RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

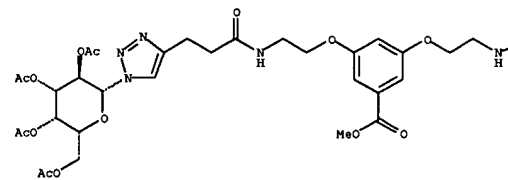
L4 ANSWER 31 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:367502 CASREACT
 TI High-yielding microwave-assisted synthesis of triazole-linked glycodendrimers by copper-catalyzed [3+2] cycloaddition
 AU Joosten, John A. F.; Tholen, Niels T. H.; El Maate, Fatma Ait; Brouwer, Arwin J.; van Esse, G. Wilma; Rijkers, Dirk T. S.; Liskamp, Rob M. J.; Pieters, Roland J.
 CS Department of Medicinal Chemistry, Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Utrecht, 3508 TB, Neth.
 SO European Journal of Organic Chemistry (2005), (15), 3182-3185
 CODEN: EJOCFK; ISSN: 1434-193X
 FB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 AB A facile and high-yielding synthesis of multivalent 1,4-disubstituted 1,2,3-triazole-linked glycodendrimers is described. Azido carbohydrates are linked by a Cu(I)-catalyzed [3+2]-cycloaddn. reaction to dendritic acetylene using microwave irradiation

RX(1) OF 34 ... 2 A + B ==> C

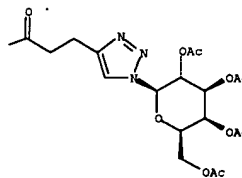


L4 ANSWER 31 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

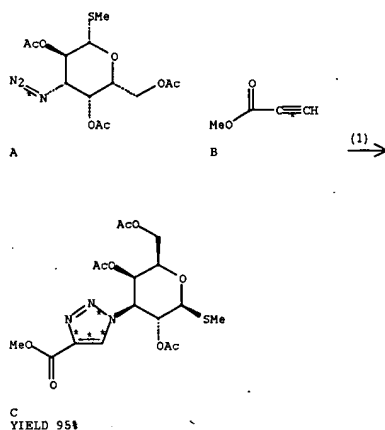


C
YIELD 93%

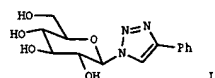
RX(1) RCT A 13992-26-2, B 866088-19-9
 RGT D 134-03-2 Na ascorbate, E 7732-18-5 Water, F 7758-98-7 CuSO₄
 PRO C 866088-25-7
 SOL 68-12-2 DMF
 CON 20 minutes, 80 deg C
 NTE microwave irradiation
 RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 32 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:230111 CASREACT
 TI 3-(1,2,3-Triazol-1-yl)-1-thio-galactosides as small, efficient, and hydrolytically stable inhibitors of galectin-3
 AU Salameh, Bader A.; Leffler, Hakon; Nilsson, Ulf J.
 CS Organic Chemistry, Lund University, Lund, SE-221 00, Sved.
 SO Bioorganic & Medicinal Chemistry Letters (2005), 15(14), 3344-3346
 CODEN: BMCLES; ISSN: 0960-894X
 PB Elsevier B.V.
 DT Journal
 LA English
 AB Copper(I)-catalyzed addition of alkynes to Me 3-azido-3-deoxy-1-thio- β -D-galactopyranoside afforded stable and structurally simple 3-deoxy-3-(1H-1,2,3-triazol-1-yl)-1-thio-galactosides carrying a panel of substituents at the triazole C4 in high yields. The 3-(1H-[1,2,3]-triazol-1-yl)-1-thio-galactoside collection synthesized contained inhibitors of the tumor- and inflammation-related galectin-3 with K_d values as low as 107 μ M, which is as potent as the natural disaccharide inhibitors lactose and N-acetylglucosamine.

RX(1) OF 27 A + B ==> C...

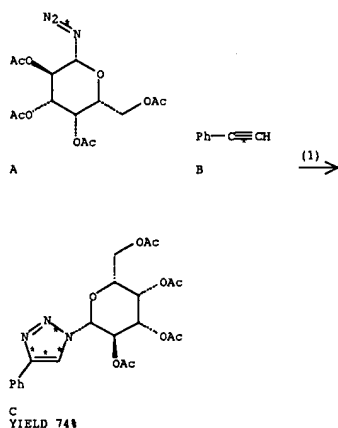


L4 ANSWER 33 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:212092 CASREACT
 TI Glycosidase inhibition by 1-glycosyl-4-phenyl triazoles
 AU Rossi, Lauren L.; Basu, Amit
 CS Department of Chemistry, Brown University, Providence, RI, 02912, USA
 SO Bioorganic & Medicinal Chemistry Letters (2005), 15(15), 3596-3599
 CODEN: BMCLES; ISSN: 0960-894X
 PB Elsevier B.V.
 DT Journal
 LA English
 GI



AB 1-Glycosyl-4-Ph triazoles, e.g. 1, have been prepared via a copper-mediated [3+2]-cycloaddn. of glycosyl azides with phenylacetylene. These triazoles have been evaluated for their ability to inhibit the enzymic activity of glycosidases.

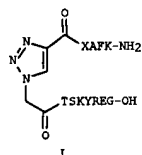
RX(1) OF 6 A + B ==> C...



L4 ANSWER 32 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 RX(1) RCT A 443864-69-5, B 922-67-8
 RGT D 7087-68-5 EtN(Pr-i)2, E 7758-89-6 CuCl
 PRO C 862670-76-6
 SOL 108-88-3 PhMe
 CON 40 deg C
 RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

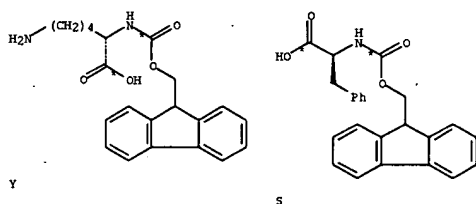
L4 ANSWER 33 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 RX(1) RCT A 13992-26-2, B 536-74-3
 RGT D 7087-68-5 EtN(Pr-i)2
 PRO C 26295-46-5
 CAT 13767-71-0 CuI2
 SOL 108-88-3 PhMe
 CON room temperature
 RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 34 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:194214 CASREACT
 TI Peptide ligation through click chemistry for the generation of assembled
 and scaffolded peptides
 AU Franke, Raimo; Doll, Christian; Eichler, Jutta
 CS German Research Centre for Biotechnology, Braunschweig, 38124, Germany
 SO Tetrahedron Letters (2005), 46(26), 4479-4482
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier B.V.
 DT Journal
 LA English
 GI



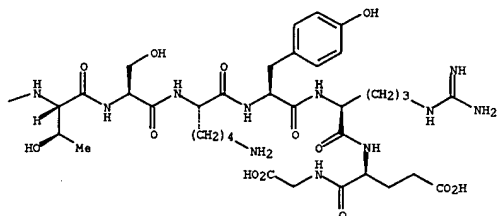
AB The synthesis of [1,2,3]-triazoles through copper(I)-catalyzed Huisgen 1,3-dipolar cycloaddn. was examined for its utility to generate assembled and scaffolded peptides from peptide and scaffold precursors, which were N-terminally modified with azido and alkyne moieties, resp. Thus, triazolyl peptides I [X = C, D, E, G, H, M, N, Q, R, S, T, W, Y (one-letter amino acid symbols)] were prepared by ligating a protected azido peptide to resin-bound alkynes HC.tplbond.CCO-XAFK-resin.

RX(5) OF 40
 AB ...Y + S + T + Z + AA + I ==>



L4 ANSWER 34 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



AB
 YIELD 71%

RX(5) RCT Y 105047-45-8

STAGE(1)
 RGT J 693-13-0 i-PrN:C:NPr-i, K 2592-95-2 1-Benzotriazolol
 SOL 68-12-2 DMF
 CON 60 minutes, room temperature

STAGE(2)
 RCT S 35661-40-6
 RGT J 693-13-0 i-PrN:C:NPr-i, K 2592-95-2 1-Benzotriazolol
 SOL 68-12-2 DMF
 CON 60 minutes, room temperature

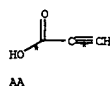
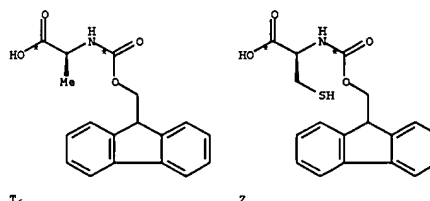
STAGE(3)
 RCT T 35661-39-3
 RGT J 693-13-0 i-PrN:C:NPr-i, K 2592-95-2 1-Benzotriazolol
 SOL 68-12-2 DMF
 CON 60 minutes, room temperature

STAGE(4)
 RCT Z 135248-89-4
 RGT J 693-13-0 i-PrN:C:NPr-i, K 2592-95-2 1-Benzotriazolol
 SOL 68-12-2 DMF
 CON 60 minutes, room temperature

STAGE(5)
 RCT AA 471-25-0
 RGT J 693-13-0 i-PrN:C:NPr-i
 SOL 75-09-2 CH2Cl2, 68-12-2 DMF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 2 hours, room temperature

STAGE(6)
 RCT I 861657-13-8
 RGT AC 7087-68-5 EtN(Pr-i)2
 CAT 7681-65-4 CuI

L4 ANSWER 34 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

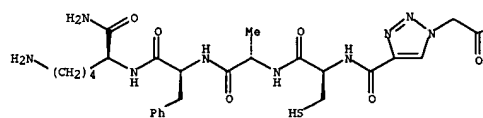


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

(5) →

PAGE 1-A



L4 ANSWER 34 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 68-12-2 DMF
 CON 2 days, room temperature

STAGE(7)

RGT AD 6485-79-6 Silane, tris(1-methylethyl)-, M 7732-18-5
 Water, N 76-05-1 F3CCO2H
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2, 76-05-1 F3CCO2H
 CON 2 hours, room temperature

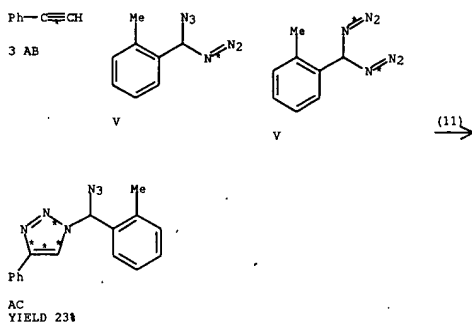
PRO AB 861656-98-6

NTE combinatorial, solid-supported reaction, first stage is attachment to TentaGel S RAM resin, Fmoc deprotection steps omitted, stage 6 in the dark and regioselective Huisgen 1,3-dipolar cycloaddition, other product also detected
 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

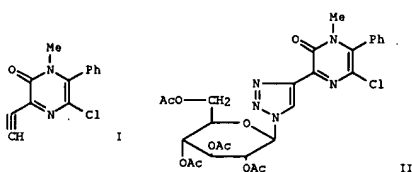
RE.CNT 14

L4 ANSWER 35 OF 69 CASREACT COPYRIGHT 2006 ACS ON STN
 AN 143:193958 CASREACT
 TI Kinetic resolution by copper-catalyzed azide-alkyne cycloaddition
 AU Meng, Jun-cai; Fokin, Valery V.; Finn, M. G.
 CS Department of Chemistry, Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Tetrahedron Letters (2005), 46(27), 4543-4546
 CODEN: TETLEA; ISSN: 0040-4039
 PB Elsevier B.V.
 DT Journal
 LA English
 AB The use of chiral pybox ligands imparts enantioselectivity to the CuI-catalyzed azide-alkyne cycloaddn. reaction, in the form of kinetic resolution of α -chiral azides and desymmetrization of gem-diazides. While levels of selectivity are modest, the results show unequivocally that the process benefits from ligand-accelerated catalysis. Some copper complexes are known to involve a copper (I)-acetylide species; a selection of pybox ligands was screened in the kinetic resolution of a racemic azides. Each showed an acceleration rate with respect to the reaction in the absence of a chelating ligand. It was shown that the ligands are involved in the copper-catalyzed process (ligand-accelerated catalysis). The cycloaddn. of 2-[1-(azido)ethyl]naphthalene with (ethynyl)benzene gave 1-[1-(2-naphthalenyl)ethyl]-4-phenyl-1,2,3-triazole.

RX(11) OF 25 ...3 AB + 2 V ==> AC + AD



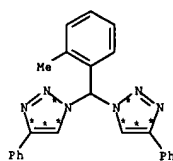
L4 ANSWER 36 OF 69 CASREACT COPYRIGHT 2006 ACS ON STN
 AN 143:153593 CASREACT
 TI Indirect coupling of the 2(1H)-pyrazinone scaffold with various (oligo)-saccharides via "click chemistry": En route towards glycopeptidomimetics
 AU Ermolat'ev, Denis; Dehaen, Wim; Van der Eycken, Erik
 CS Laboratory for Organic Synthesis, Department of Chemistry, University of Leuven, Louvain, B-3001, Belg.
 SO QSAR & Combinatorial Science (2004), 23(10), 915-918
 CODEN: QCSAUI; ISSN: 1611-020X
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 GI



AB The indirect coupling via a 1,2,3-triazole ring system, of the 2(1H)-pyrazinone scaffold with various saccharides is described. A microwave-enhanced Cu(I)-catalyzed Huisgen [2 + 3] dipolar cycloaddn. reaction was applied. E.g., 3-ethynylpyrazinone derivative I was reacted with 2,3,4,6-tetra-O-acetyl- β -D-glucopyranosyl azide in the presence of Cu turnings, CuSO₄ and N,N,N-tris[1-(benzyl)-1H-1,2,3-triazol-4-yl]methylamine in THF/H₂O and using microwave irradiation to give cycloaddn. product II in 89% yield. This opens the way for the generation of an interesting new class of glycopeptidomimetics.

RX(1) OF 17 A + B ==> C...

L4 ANSWER 35 OF 69 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



AD
 YIELD 60%

RX(11) RCT AB 536-74-3

STAGE(1)

CAT 862080-12-4 1H-Indole, 3,3'-[2,6-pyridinediylbis[(4S)-4,5-dihydro-2,4-oxazolediyl]methylene]bis-, 7681-65-4 CuI
 SOL 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) 10 minutes, room temperature
 SUBSTAGE(2) 30 minutes, room temperature
 SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

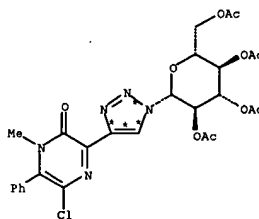
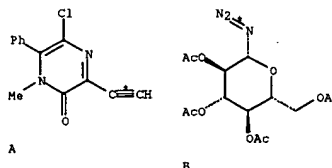
RCT V 143468-04-6
 CAT 7087-68-5 EtN(Pr-i)2
 SOL 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 24 hours, 0 - 4 deg C

PRO AC 862080-13-5, AD 862080-14-6

NTE stereoselective

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 36 OF 69 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



C
 YIELD 89%

RX(1) RCT A 859845-35-5, B 13992-25-1

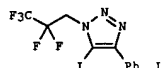
PRO C 859845-36-6

CAT 7440-50-8 Cu, 7758-98-7 CuSO₄, 510758-28-8 1H-1,2,3-Triazole-4-methanamine, 1-(phenylmethyl)-N,N-bis[1-(phenylmethyl)-1H-1,2,3-triazol-4-yl]methyl]-
 SOL 7732-18-5 Water, 109-99-9 THF
 CON 8 minutes, 85 deg C

NTE microwave irradian., regioselective, Huisgen [3+2] dipolar cycloaddition, in-situ generated catalyst

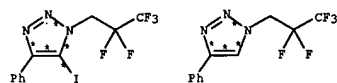
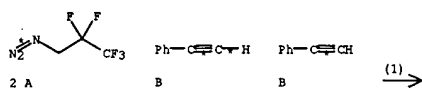
RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 37 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:153330 CASREACT
 T1 Regiospecific synthesis of 1,4,5-trisubstituted-1,2,3-triazoles via one-pot reaction promoted by copper(I) salt
 AU Wu, Yong-Ming; Deng, Juan; Li, Ya; Chen, Qing-Yun
 CS Key Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
 SO Synthesis (2005), (8), 1314-1318
 CODEN: SYNTBF; ISSN: 0039-7881
 PB Georg Thieme Verlag
 DT Journal
 LA English
 GI



AB A method for the regiospecific synthesis of 1,4,5-trisubstituted-1,2,3-triazoles, e.g., 1, catalyzed by copper(I) iodide was developed. This is an example of a regiospecific synthesis of 5-iodo-1,4-disubstituted-1,2,3-triazoles, which can be further elaborated to a range of 1,4,5-trisubstituted-1,2,3-triazole derivs.

RX(1) OF 22 2 A + 2 B ==> C + D

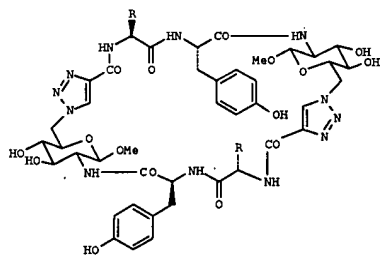


C
YIELD 42%

D
YIELD 48%

RX(1) RCT A 860002-53-5, B 536-74-3
 RGT E 7681-65-4 CuI, F 121-44-8 Et3N, G 7553-56-2 I2
 PRO C 860002-54-6, D 860002-55-7
 SOL 75-05-9 MeCN
 CON 20 hours, room temperature

L4 ANSWER 38 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:115781 CASREACT
 T1 C2-Symmetric Macrocyclic Carbohydrate/Amino Acid Hybrids through Copper(I)-Catalyzed Formation of 1,2,3-Triazoles
 AU Billing, Johan F.; Nilsson, Ulf J.
 CS Organic Chemistry, Lund University, Lund, SE-221 00, Swed.
 SO Journal of Organic Chemistry (2005), 70(12), 4847-4850
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 GI

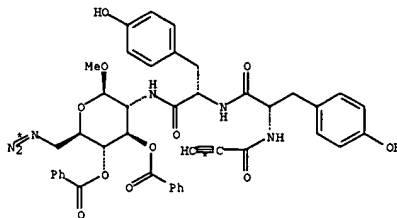


AB An efficient method was developed for the preparation of macrocyclic carbohydrate/amino acid hybrids I [R = CH2C6H4OH-4, (CH2)3NHC(=NH)NH2] by macrocyclization with copper(I)-catalyzed 1,2,3-triazole formation. Me 2-amino-6-azido-3,4-di-O-benzoyl-2,6-dideoxy-β-D-glucopyranoside was prepared and coupled to two different N-propionyl dipeptides [HC.tpbond.CO-Tyr-Tyr-OH and HC.tpbond.CO-Arg(Mtr)-Tyr-OH] to obtain bifunctional mols. carrying one azido group and one terminal alkyne. These bifunctional mols. were cyclodimerized using Cu(I)-catalyzed 1,3-dipolar cycloaddn. of azides and alkynes to form macrocycles containing two 1,2,3-triazoles. Various cyclization methods were evaluated, and the most efficient conditions were found to be CuI and N,N-diisopropylethylamine in CH3CN.

RX(12) OF 130 ...2 AC ==> AH...

L4 ANSWER 37 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 NTE regiospecific
 RE.CMT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 38 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2 AC

(12)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A

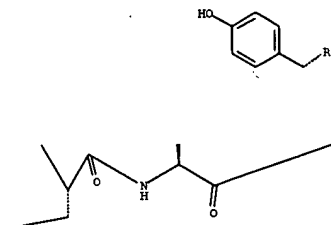
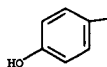
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-C

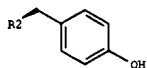


L4 ANSWER 38 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 3-A



PAGE 3-B



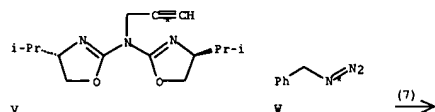
PAGE 4-A

AH
YIELD 64%

RX(12) RCT AC 857351-81-6
RGT AI 7681-65-4 CuI, AJ 7087-68-5 EtN(Pr-i)2
PRO AH 857351-83-8

L4 ANSWER 39 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
AN 143:97144 CASREACT
TI Cu(II)-Aza(bisoxazoline)-Catalyzed Asymmetric Benzoylations
AU Gissibl, Anja; Finn, M. G.; Reiser, Oliver
CS Institut fuer Organische Chemie, Universitaet Regensburg, Regensburg,
D-93053, Germany
SO Organic Letters (2005), 7(12), 2325-2328
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
AB Racemic 1,2-diols and α -hydroxy carbonyl compds. can be asym.
benzoylated in a kinetic resolution in the presence of various
Cu(II)-aza(bisoxazoline) catalysts. A novel bis benzyl-substituted
aza(bisoxazoline) ligand proved to be especially effective when immobilized
on MeOPEG5000, giving from 91 to 29% ee in 37-49% yield for each of
five sequential reactions.

RX(7) OF 36 ...V + W ==> X

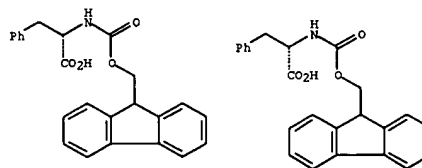
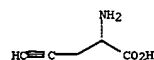
X
YIELD 78%

RX(7) RCT V 856899-72-4, W 622-79-7
RGT Y 134-03-2 Na ascorbate, Z 7758-98-7 CuSO4
PRO X 856899-73-5
SOL 7732-18-5 Water, 75,65-0 t-BuOH
CON 20 hours, room temperature
NTE solid-supported reaction
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 38 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

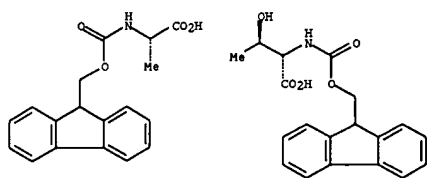
SOL 75-05-8 MeCN
CON 72 hours, 45 deg C
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 40 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
AN 143:60234 CASREACT
TI Head-to-tail peptide cyclodimerization by copper-catalyzed
azide-alkyne cycloaddition
AU Punna, Sreenivas; Kuzelka, Jane; Wang, Qian; Finn, M. G.
CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
92037, USA
SO Angewandte Chemie, International Edition (2005), 44(15), 2215-2220
CODEN: ACHIE5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB Oligopeptide cyclodimerization occurs selectively when precursors containing
azide and alkyne groups are exposed to copper(I) ions on
polystyrene supports. Thus, resin-bound 11- and 19-mer Arg-Gly-Asp (RGD)
peptides containing L-propargylglycine as second residue and
5-azidopentanoyl-capped lysine N-terminus were treated with CuI for 16 h
to effect cyclodimerization via formation of two triazole rings.

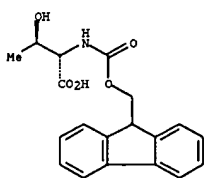
RX(2) OF 8 2 A + B + C + D + E + F + G + H + I +
J ==> PA
resin bound

B

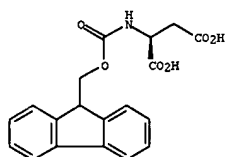
L4 ANSWER 40 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



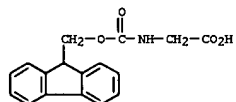
C



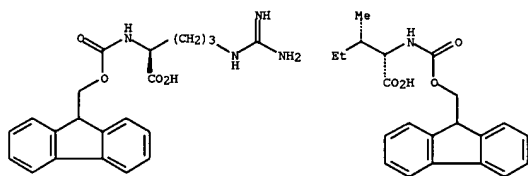
D



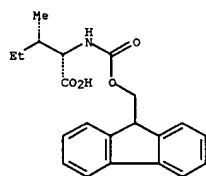
E



F



G



H

L4 ANSWER 40 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RGT M 71989-23-6

STAGE(10)

RGT I 71989-26-9

STAGE(11)

RGT J 79583-98-5

STAGE(12)

RGT Q 540-63-6 HSCH2CH2SH, R 7681-65-4 CuI, S 108-48-5

2,6-Lutidine

SOL 7732-18-5 Water, 75-05-8 MeCN, 67-68-5 DMSO

CON 16 hours, room temperature

STAGE(13)

RGT L 6485-79-6 Silane, tris(1-methylethyl)-, M 7732-18-5

Water, N 76-05-1 F3CCO2H

SOL 76-05-1 F3CCO2H

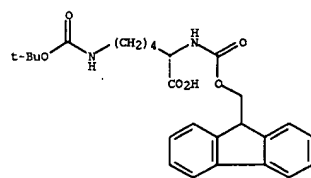
CON 3 hours, room temperature

PRO P 853889-18-6

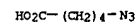
NTE solid-supported reaction, supported on Wang resin, standard Fmoc based solid-phase peptide synthesis, alternate preparation using Boc-based protocol described

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 40 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



I



J

(2) →

STRUCTURE
DIAGRAM
IS NOT
AVAILABLEP
YIELD 20%

RX(2) RCT A 35661-40-60

STAGE(1)

STAGE(2)

RCT B 23235-01-0

STAGE(3)

RCT C 35661-39-3

STAGE(4)

RCT O 35661-40-6

STAGE(5)

RCT D 73731-37-0

STAGE(6)

RCT E 119062-05-4

STAGE(7)

RCT F 29022-11-5

STAGE(8)

RCT G 91000-69-0

STAGE(9)

L4 ANSWER 41 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 143:43833 CASREACT

T1 The Application of "Click Chemistry" for the Decoration of

2(1H)-Pyrazinone Scaffold: Generation of Templates

AU Kaval, Nadya; Ermolat'ev, Denis; Appukkuttan, Prasad; Dehaen, Wim; Kappe,

C. Oliver; Van der Eycken, Erik

CS Laboratory for Organic Synthesis, University of Leuven, Louvain, B-3001,

Belg.

SO Journal of Combinatorial Chemistry (2005), 7(3), 490-502

CODEN: JCCHFF; ISSN: 1520-4766

PB American Chemical Society

DT Journal

LA English

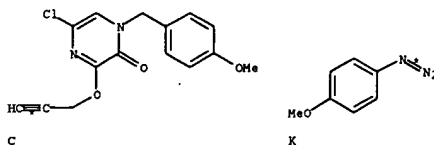
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The "click chemical" approach has been explored on the 2(1H)-pyrazinone scaffold for the generation of pharmacol. interesting heterocyclic moieties. Huisgen 1,3-dipolar cycloaddn. has been evaluated as the key step for the construction of the 1,2,3-triazole ring at the C-3 position of 2(1H)-pyrazinones. Two different pathways have been successfully evaluated: (1) via C-C or C-O linkage of the acetylenic part to the C-3 position of the 2(1H)-pyrazinone scaffold or (2) via azide introduction in the C-3 position. The subsequent application of "click chemical" resulted

in the formation of hitherto unknown skeletons. Microwave irradiation has successfully been applied in different steps of the sequence. E.g., microwave-enhanced 1,3-dipolar cycloaddn. of acetylene-functionalized 2(1H)-pyrazinone I with 4-MeOC6H4N3 gave triazolyl-substituted pyrazinone II. Microwave-enhanced Diels-Alder reaction of II with DMAP gave pyridine derivative III. Alternatively, microwave-enhanced 1,3-dipolar cycloaddn. of tetrazole derivative IV with phenylacetylene gave triazole derivative V.

RX(3) OF 116 ...C + K ==> L...

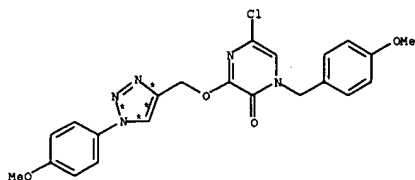


C

K

(3) →

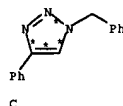
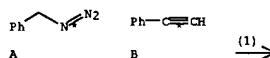
L4 ANSWER 41 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L
YIELD 84%

RX(3) RCT C 853192-69-5, K 2101-87-3
 PRO L 853192-71-9
 CAT 7440-50-8 Cu, 7758-98-7 CuSO₄, 853193-06-3 1H-1,2,3-Triazole-4-ethanamine, 1-(phenylmethyl)-N,N-bis[2-[1-(phenylmethyl)-1H-1,2,3-triazol-4-yl]ethyl]-
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 0.5 minutes, 100 deg C
 NTE microwave irradiation, regioselective, alternative reaction conditions gave lower yield
 RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

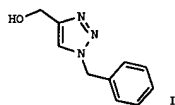
L4 ANSWER 42 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 143:26152 CASREACT
 TI Mechanism of the ligand-free CuI-catalyzed azide-alkyne cycloaddition reaction
 AU Rodionov, Valentin O.; Fokin, Valery V.; Finn, M. G.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Angewandte Chemie, International Edition (2005), 44(15), 2210-2215
 CODEN: ACIEF5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 AB The Cu-catalyzed azide-alkyne cycloaddn. depends on rapid formation of CuI-acetylide complexes from terminal alkynes and their ability to activate organic azides. A kinetics study uncovered a bimol. dependence on the metal and an unusually fast intramol. variant of the process.

RX(1)-OF 3 A + B ==> C



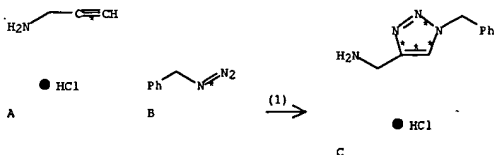
RX(1) RCT A 622-79-7, B 536-74-3
 RGT D 134-03-2 Na ascorbate
 PRO C 108717-96-0
 CAT 7758-98-7 CuSO₄
 SOL 7732-18-5 Water, 67-68-5 DMSO
 CON 20+/-2 deg C
 RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 43 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:481993 CASREACT
 TI Regioselective synthesis of [1,2,3]-triazoles catalyzed by Cu(I) generated in situ from Cu(0) nanosize activated powder and amine hydrochloride salts
 AU Orqueira, Hernan A.; Fokas, Demosthenes; Isome, Yuko; Chan, Philip C.-M.; Baldino, Carmen M.
 CS Department of Chemistry, ArQuile, Inc., Woburn, MA, 01801, USA
 SO Tetrahedron Letters (2005), 46(16), 2911-2914
 CODEN: TETLEY; ISSN: 0040-4039
 PB Elsevier B.V.
 DT Journal
 LA English
 GI



AB A straightforward and efficient method for the regioselective synthesis of functionalized 1,4-disubstituted [1,2,3]-triazoles, e.g., I, from terminal alkynes and azides, has been established utilizing Cu(0) as the source of the catalytic species. The presumed catalytic Cu(I) species was generated by the combination of catalytic amount of copper nanosize activated powder and an equivalent of an amine hydrochloride salt. The addition of an amine hydrochloride salt into the reaction mixture enhanced the dissoln. of copper metal, and subsequently facilitated the formation of the Cu(I)-acetylide intermediate required for the regioselective cycloaddn.

RX(1) OF 16 A + B ==> C

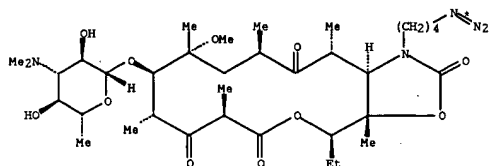


RX(1) RCT A 15430-52-1, B 622-79-7
 RGT D 554-68-7 Et3N-HCl
 PRO C 852030-90-1
 CAT 7440-50-8 Cu
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 2 hours, room temperature

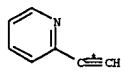
L4 ANSWER 43 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 NTE regioselective
 RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 44 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:374048 CASREACT
 TI An efficient entry to new sugar modified ketolide antibiotics
 AU Romero, Alex; Liang, Chang-Hsing; Chiu, Yu-Hung; Yao, Sulan; Duffield, Jonathan; Sucheck, Steven J.; Marby, Ken; Rabuka, David; Leung, Po Yee; Shue, Youe-Kong; Ichikawa, Yoshi Hwang, Chan-Kou
 CS Department of Chemistry, Optimer Pharmaceuticals, Inc., San Diego, CA, 92121, USA
 SO Tetrahedron Letters (2005), 46(9), 1483-1487
 CODEN: TETLEA; ISSN: 0040-4039
 PB Elsevier B.V.
 DT Journal
 LA English
 AB A new and efficient route to a ketolide aglycon served as a basis for the unprecedented 5-O-glyco-modification of ketolide antibiotics. Combined with an effective copper-catalyzed triazole-forming reaction a series of novel and potent ketolide antibiotics were synthesized.

RX(21) OF 174 ...AR + AU ==> AV



AR

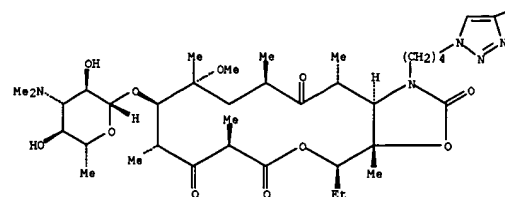


AU

(21)

L4 ANSWER 44 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

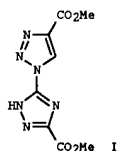


AV
YIELD 98%

RX(21) RCT AR 760981-88-2, AU 1945-84-2
 PRO AV 849407-88-1
 CAT 7681-65-4 CuI
 SOL 108-88-3 PhMe
 CON 75 deg C

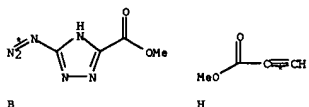
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 45 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:373763 CASREACT
 TI Synthesis of bitriazolyl compounds via Huisgen reaction
 AU Xia, Yi; Qu, Fangqi; Li, Wei; Wu, Qiongyou; Peng, Ling
 CS College of Chemistry and Molecular Sciences, Wuhan University, Wuhan, 430072, Peop. Rep. China
 SO Heterocycles (2005), 65(2), 345-352
 CODEN: HETCYM; ISSN: 0385-8144
 PB Japan Institute of Heterocyclic Chemistry
 DT Journal
 LA English
 GI



AB Bitriazolyl compds. were synthesized via Huisgen 1,3-cycloaddn. starting with an (azido)triazole and various alkynes. Good yields were obtained with terminal alkynes using copper(I) as a catalyst in the THF/H₂O system. For example, the cycloaddn. of 5-(azido)-1H-1,2,4-triazole-3-carboxylic Me ester with 2-propynoic acid Me ester gave a bitriazole, [4-(methoxycarbonyl)-1H-1,2,3-triazol-1-yl]-1H-1,2,4-triazole-4-carboxylic acid Me ester (I), (isolated isomer) in 81.2% yield.

RX(2) OF 26 ...B + H ==> I

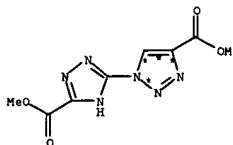


B

H

(2)

L4 ANSWER 45 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



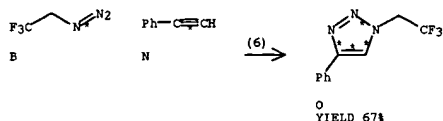
I
YIELD 75%

RX(2) RCT B 53566-46-4, H 922-67-8
 PRO I 849339-73-7
 SOL 108-88-3 PhMe
 CON 55 hours, 120 deg C
 NTE regioselective

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 46 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:261471 CASREACT
 TI Regioselective synthesis of fluoroalkylated [1,2,3]-triazoles by Huisgen cycloaddition
 AU Wu, Yong-Ming; Deng, Juan; Fang, Xiang; Chen, Qing-Yun
 CS Shanghai Institute of Organic Chemistry, Key Laboratory of Organofluorine Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
 SO Journal of Fluorine Chemistry (2004), 125(10), 1415-1423
 CODEN: JFLCAR; ISSN: 0022-1139
 PB Elsevier B.V.
 DT Journal
 LA English
 AB A series of fluoroalkylated 1,4-disubstituted [1,2,3]-triazoles were synthesized by the 1,3-dipolar cycloaddn. of fluoroalkylated azides with terminal alkynes in the presence of Cu(I) salt as catalyst at room temperature
 All the reactions were highly regioselective; no 1,5-disubstituted product was formed. For aryl- or alkylalkynes, triethylamine should be used as ligand. But for propiolic ester(amide), addition of triethylamine gave no products. A mechanism of Cu(I) inserting the internal alkyne was suggested.

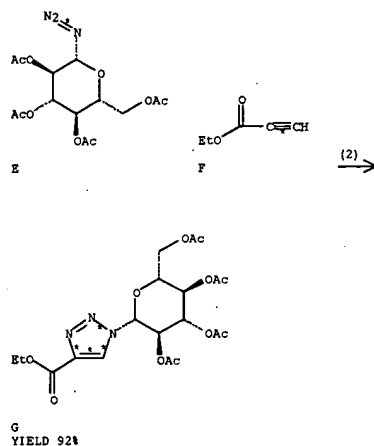
RX(6) OF 61 ...B + N ==> O



RX(6) RCT B 846057-92-9, N 536-74-3
 RGT P 121-44-8 Et3N
 PRO O 846057-98-5
 CAT 7681-65-4 CuI
 SOL 7732-18-5 Water, 75-05-8 MeCN
 CON 20 hours, room temperature
 NTE regioselective, Huisgen reaction, optimization study(optimized on solvent, temperature, presence or absence of reagent, presence or absence of catalyst)
 RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 47 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:240643 CASREACT
 TI Rapid access to glucopyranosyl-1,2,3-triazoles via Cu(I)-catalyzed reactions in water
 AU Akula, Rakesh A.; Temelkoff, David P.; Artis, Nicole D.; Norris, Peter
 CS Department of Chemistry, Youngstown State University, Youngstown, OH, 44555, USA
 SO Heterocycles (2004), 63(12), 2719-2725
 CODEN: HETCYM; ISSN: 0385-5414
 PB Japan Institute of Heterocyclic Chemistry
 DT Journal
 LA English
 AB 1-Azido-1-deoxy-2,3,4,6-tetra-O-acetyl-β-D-glucopyranose reacts with various terminal alkynes in the presence of CuSO4/ascorbic acid in water to give the corresponding 1,4-disubstituted 1,2,3-triazoles, which are isolated in high yield and purity by simply filtering the precipitate from the reaction mixture. Several sugar-derived acetylenes react similarly to yield triazole-linked disaccharide analogs.

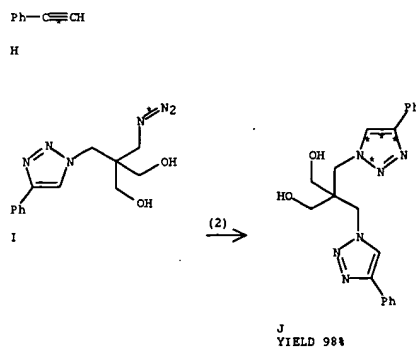
RX(2) OF 16 E + F ==> G



L4 ANSWER 47 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 RX(2) RCT E 13992-25-1, F 623-47-2
 RGT H 82624-30-0 Ascorbic acid
 PRO G 844864-81-9
 CAT 7758-98-7 CuSO4
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 8 hours, 70 deg C
 SUBSTAGE(2) 70 deg C -> room temperature
 RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 48 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:176314 CASREACT
 TI Copper(I)-Catalyzed Synthesis of Azoles. DFT Study Predicts Unprecedented Reactivity and Intermediates
 AU Himo, Fahmi; Lovell, Timothy; Hilgraf, Robert; Rostovtsev, Vsevolod V.; Noodleman, Louis; Sharpless, K. Barry; Fokin, Valery V.
 CS Department of Molecular Biology and Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Journal of the American Chemical Society (2005), 127(1), 210-216
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB Huisgen's 1,3-dipolar cycloaddns. become nonconcerted when copper (I) acetylides react with azides and nitrile oxides, providing ready access to 1,4-disubstituted 1,2,3-triazoles and 3,4-disubstituted isoxazoles, resp. The process is highly reliable and exhibits an unusually wide scope with respect to both components. Computational studies revealed a stepwise mechanism involving unprecedented metallacycle intermediates, which appear to be common for a variety of dipoles.

RX(2) OF 24 H + I ==> J



RX(2) RCT H 536-74-3, I 834894-31-4
 PRO J 478555-24-7
 CAT 7440-50-8 Cu
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 24 hours
 NTE regioselective
 RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

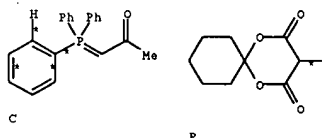
L4 ANSWER 48 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L4 ANSWER 49 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:93753 CASREACT
 TI Towards organo-click chemistry: Development of organocatalytic multicomponent reactions through combinations of Aldol, Wittig, Knoevenagel, Michael, Diels-Alder and Huisgen cycloaddition reactions
 AU Ramachary, Dhevalapally B.; Barbas, Carlos F., III
 CS Departments of Chemistry and Molecular Biology and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Chemistry--A European Journal (2004), 10(21), 5323-5331
 CODEN: CEUJED; ISSN: 0947-6539
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 GI

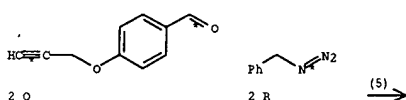
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Studies on multicomponent reactions (MCRs) catalyzed by combinations of amino acids and copper(I) are reported. Exptl. simple and environmentally friendly, organocatalytic, asym. four-component Diels-Alder (AFCD) reactions of 1-(triphenylphosphanylidene)-propan-2-one, two different aldehydes, and cyclic 1,3-diketones produced diastereospecific and highly enantioselective substituted spirotriones, e.g., I, by means of a Wittig/Knoevenagel/Diels-Alder reaction sequence in one pot. Chemical diversity libraries of polysubstituted spirotrione-1,2,3-triazoles, e.g., II, were assembled from simple substrates by means of Wittig/Knoevenagel/Diels-Alder/Huisgen cycloaddn. reaction sequences in one pot under stereospecific organo/CuI catalysis. Functionalized dispirolactones such as III (Ar = 4-HOC6H4), are biol. active antioxidants and radical scavengers, and spirotrione-1,2,3-triazoles have found wide applications in chemical, biol., and materials science. Addnl. an organocatalytic, asym. three-component Michael (ATCM) reaction of 1-(triphenylphosphanylidene)-propan-2-one, aldehyde, and cyclic 1,3-diketones was developed that produced Michael adducts IV (R = Et, Ar = Bu; R = Bu, Ar = 2-NO2C6H4) through a Wittig/Michael reaction sequence in a highly enantioselective one-pot process.

RX(5) OF 40 C + P + 2 Q + 2 R ==> S

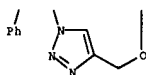


L4 ANSWER 49 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



S
 YIELD 90%

RX(5) ACT C 1439-36-7, P 1658-27-1, Q 5651-86-5

STAGE(1)

CAT 147-85-3 (S)-Proline
 SOL 64-17-5 EtOH
 CON 3 - 12 hours, 65 deg C

STAGE(2)

RCT R 622-79-7
 CAT 7440-50-8 Cu, 7758-98-7 CuSO4
 CON 15 - 48 hours, room temperature

PRO S 817206-77-2

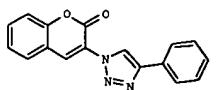
NTE regioselective, stereoselective, Huisgen cycloaddition step 2,
 domino Wittig/Knoevenagel/Diels-Alder reaction step 1
 RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 50 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 142:93748 CASREACT
 TI A Fluorogenic 1,3-Dipolar Cycloaddition Reaction of 3-Azidocoumarins and Acetylenes

AU Sivakumar, Krishnamoorthy; Xie, Fang; Cash, Brandon M.; Long, Su; Barnhill, Hannah N.; Wang, Qian
 CS Department of Chemistry Biochemistry, University of South Carolina, Columbia, SC, 29208, USA

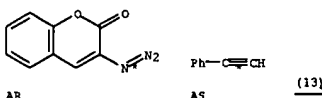
SO Organic Letters (2004), 6(24), 4603-4606
 CODEN: ORLEF7; ISSN: 1522-7060

PB American Chemical Society
 DT Journal
 LA English
 GI



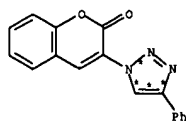
AB Fluorescent 1-coumarinyl-1,2,3-triazoles such as I are prepared by regioselective 1,3-dipolar cycloaddn. of coumarinyl azides and aryl alkynes in the presence of copper (II) sulfate and sodium ascorbate. E.g., 3-azido-2H-benzopyran-2-one undergoes 1,3-dipolar cycloaddn. with phenylacetylene in ethanol/water in the presence of copper (II) sulfate and sodium ascorbate to yield I in 81% yield after recrystn. (100% yield by NMR); I absorbs light at 340 nm and emits fluorescence at 478 nm. A combinatorial library is prepared by the reactions of ten coumarinyl azides with 24 alkynes; for some of the products, yields and NMR or m.p. data are obtained, while for most of the products the fluorescence excitation and emission wavelengths are determined. Most of the products are fluorescent and have potential utility as fluorescent dyes; the effectiveness of the dipolar cycloaddn. reaction at low temps. (0°) and the inertness of the reagents allows for its potential use as a labeling method for biol. systems.

RX(13) OF 498 AR + AS ==> AT



L4 ANSWER 50 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

AT
YIELD 100%

RX(13) RCT AR 152711-55-2, AS 536-74-3
 PRO AT 817638-77-0
 CAT 7758-98-7 CuSO₄, 134-03-2 Na ascorbate
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON 24 hours, room temperature
 NTE combinatorial, regioselective
 RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 51 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 142:56242 CASREACT

TI A microwave-assisted click chemistry synthesis of 1,4-disubstituted 1,2,3-triazoles via a copper(I)-catalyzed three-component reaction

AU Appukkuttan, Prasad; Dehaen, Wim; Fokin, Valery V.; Van der Eycken, Erik

CS Department of Chemistry, University of Leuven, Louvain, B-3001, Belg.

SO Organic Letters (2004), 6(23), 4223-4225

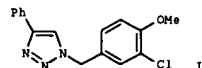
CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

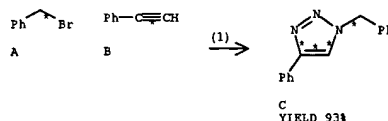
LA English

GI



AB A microwave-assisted three-component reaction was used to prepare a series of 1,4-disubstituted-1,2,3-triazoles, e.g., I, from corresponding alkyl halides, sodium azide, and alkynes. This procedure eliminated the need to handle organic azides, as they were generated in situ, making this already powerful click process even more user-friendly and safe.

RX(1) OF 14 A + B ==> C

C
YIELD 93%

RX(1) RCT A 100-39-0, B 536-74-3
 RGT D 26628-22-8 NaN₃
 PRO C 108717-96-0
 CAT 7758-98-7 CuSO₄, 7440-50-8 Cu
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON SUBSTAGE(1) 10 minutes, 125 deg C
 SUBSTAGE(2) 60 - 120 seconds, 125 deg C -> 50 deg C
 NTE combinatorial, in-situ generated catalyst, microwave irradiation, regioselective, in-situ generated reactant, multicomponent variant of Huisgen 1,3-dipolar cycloaddition, alternate preparation described
 RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 51 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

L4 ANSWER 52 OF 69 CASREACT COPYRIGHT 2006 ACS on STN

AN 142:38512 CASREACT

TI A Chemoenzymatic Approach to Glycopeptide Antibiotics

AU Lin, Hening; Walsh, Christopher T.

CS Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA

SO Journal of the American Chemical Society (2004), 126(43), 13998-14003

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

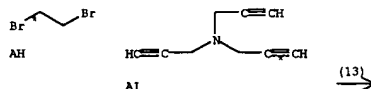
LA English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Many biol. active natural products are constrained by macrocyclization and modified with carbohydrates. These two types of modifications are essential for their biol. activities. Here we report a chemoenzymic approach to make carbohydrate-modified cyclic peptide antibiotics. Using a thioesterase domain from the decapeptide tyrocidine synthetase, 13 head-to-tail cyclized tyrocidine derivs. were obtained (no data) with one to three propargylglycines incorporated at positions 3-8. These cyclic peptides were then conjugated to 21 azido sugars via copper (I)-catalyzed cycloaddn. Antibacterial and hemolytic assays showed that the two best glycopeptides, 1 [R = CO(CH₂)₇Me, 4-PhC₆H₄(CH₂)₂], have a 6-fold better therapeutic index than the natural tyrocidine. We believe this method will also be useful for modifying other natural products to search for new therapeutics.

RX(13) OF 150 AH + AI ==> AJ...

AJ
YIELD 20%

RX(13) RCT AH 106-93-4

STAGE(1)

RCT Z 26628-22-8 NaN₃

SOL 7732-18-5 Water, 67-56-1 MeOH

CON SUBSTAGE(1) overnight, 45 deg C

L4 ANSWER 52 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
SUBSTAGE(2) 45 deg C -> room temperature

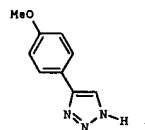
STAGE(2)

RCT AI 6921-29-5
RGT AK 134-03-2 Na ascorbate
CAT 7758-98-7 CuSO4
CON 6 hours, room temperature

PRO AJ 804557-84-4

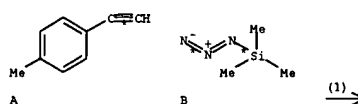
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 53 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
AN 141:424152 CASREACT
TI Copper-catalyzed synthesis of N-unsubstituted 1,2,3-triazoles from nonactivated terminal alkynes
AU Jin, Tienan; Kamijo, Shin; Yamamoto, Yoshinori
CS Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, 980-8578, Japan
SO European Journal of Organic Chemistry (2004), (18), 3789-3791
CODEN: EJOCHF; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
GI

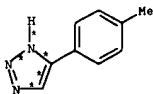


AB The [3 + 2]-cycloaddn. of nonactivated terminal alkynes and trimethylsilyl azide proceeded smoothly in the presence of CuI catalyst to give N-unsubstituted triazoles, e.g., I, in good to high yields. The reaction most probably proceeded through the in situ formation of a copper acetylide species and hydrazoic acid, followed by a successive [3 + 2]-cycloaddn. reaction.

RX(1) OF 12 A + B ==> C



L4 ANSWER 53 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

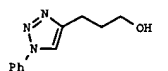


C
YIELD 83%

RX(1) RCT A 766-97-2, B 4648-54-8
PRO C 5301-96-2
CAT 7681-65-4 CuI
SOL 67-56-1 MeOH, 68-12-2 DMF
CON 12 hours, 100 deg C

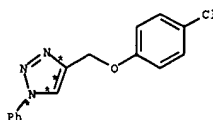
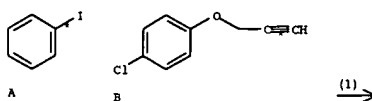
NTE optimization study, optimized on catalyst and solvent
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 54 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
AN 141:410876 CASREACT
TI One-Pot Synthesis of 1,4-disubstituted 1,2,3-triazoles from in situ generated azides
AU Feldman, Alina K.; Colasson, Benoit; Fokin, Valery V.
CS Department of Chemistry and the Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
SO Organic Letters (2004), 6(22), 3897-3899
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
GI



AB 1,4-Disubstituted 1,2,3-triazoles, e.g., I, were obtained in excellent yields by a convenient one-pot procedure, from a variety of readily available aromatic and aliphatic halides, without isolation of potentially unstable organic azide intermediates.

RX(1) OF 19 A + B ==> C



C
YIELD 83%

RX(1) RCT A 591-50-4, B 19130-39-3

STAGE(1)

RGT D 147-85-3 (S)-Proline, E 134-03-2 Na ascorbate, F 497-19-8 Na2CO3, G 26628-22-8 NaN3

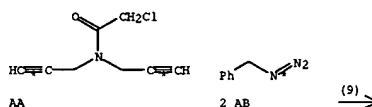
L4 ANSWER 54 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 CAT 7758-98-7 CuSO4
 SOL 7732-18-5 Water, 67-68-5 DMSO
 CON overnight, 65 deg C

STAGE(2)
 RGT H 1336-21-6 NH4OH
 SOL 7732-18-5 Water

PRO C 135034-73-0
 NTE regioselective, safety, copper azide are explosive
 RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 55 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 141:314727 CASREACT
 TI Efficiency and fidelity in a click-chemistry route to triazole dendrimers by the copper(I)-catalyzed ligation of azides and alkynes
 AU Wu, Peng; Feldman, Alina K.; Nugent, Anne K.; Hawker, Craig J.; Scheel, Arnulf; Voit, Brigitte; Pyun, Jeffrey; Frechet, Jean M. J.; Sharpless, K. Barry; Fokin, Valery V.
 CS IEM Almaden Research Center, San Jose, CA, 95120, USA
 SO Angewandte Chemie, International Edition (2004), 43(30), 3928-3932
 CODEN: ACP5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 AB A large number of diverse dendrimers was prepared with high purity in almost quant. yield by the click-chemical transformation in copper (I)-catalyzed synthesis of 1,2,3-triazoles from azides and alkynes. In some cases filtration or solvent extraction was the only method required for purification in the highly efficient construction of the triazole units of the dendrimers. Frechet's convergent approach was utilized in dendrimer synthesis; thus, the individual branches or dendron were built sequentially, starting on the outside of the mol., and they were then coupled to a multivalent centerpiece (core) in the last step.

RX(9) OF 26 AA + 2 AB ==> AC



AC
 YIELD 96%

RX(9) RCT AA 2315-38-0, AB 622-79-7

STAGE(1)
 RGT AD 7758-98-7 CuSO4, AE 134-03-2 Na ascorbate

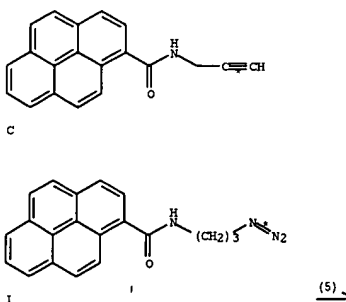
L4 ANSWER 55 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 SOL 75-65-0 t-BuOH, 75-09-2 CH2Cl2
 CON overnight, room temperature

STAGE(2)
 RGT AF 1336-21-6 NH4OH
 SOL 7732-18-5 Water
 CON 10 minutes, room temperature

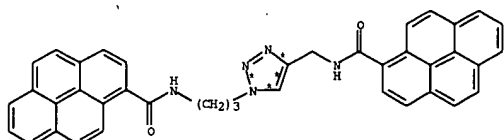
PRO AC 769387-57-1
 RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 56 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 141:309959 CASREACT
 TI FRET induced by an allosteric' cycloaddition reaction regulated with exogenous inhibitor and effectors
 AU Zhu, Lei; Lynch, Vincent M.; Anslyn, Eric V.
 CS Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712, USA
 SO Tetrahedron (2004), 60(34), 7267-7275
 CODEN: TETRA; ISSN: 0040-4020
 PB Elsevier B.V.
 DT Journal
 LA English
 AB A Cu(I) catalyzed Huisgen cycloaddn. was engineered to afford products featuring intramol. excimer formation (exciplex, 3) or intramol. Forster resonance energy transfer (FRET, 6, 7). It was further demonstrated that this reaction could be silenced by EDTA, which prohibited the reduction of copper(II) sulfate to the catalytically active Cu(I) species by sodium ascorbate. Exogenous transition metal ions such as Zn2+ and Pb2+ were shown to competitively coordinate with EDTA thus releasing free Cu2+ for the subsequent reduction, and consequently restoring the reaction. The modulated catalysis showed metal ion concentration dependence and could be monitored by both HPLC and fluorescence. This study is a demonstration of a new sensing paradigm, where a catalytic organometallic reaction can be used as the signal amplifying module of a sensing application by engineering a regulatory element into the reaction process, analogous to an allosteric enzyme or an allosteric ribozyme system.

RX(5) OF 16 ...C + I ==> M



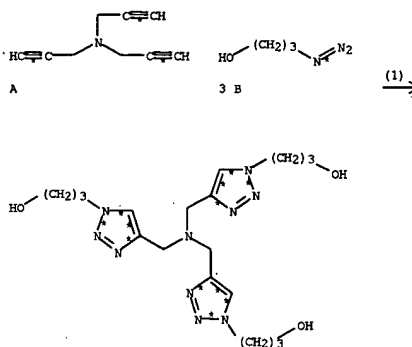
L4 ANSWER 56 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

M
YIELD 70%

RX(5) RCT C 500783-43-7, I 766536-70-3
 RGT N 134-03-2 Na ascorbate, O 7758-98-7 CuSO4
 PRO M 766536-71-4
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON 24 hours, room temperature
 RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 57 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 141:277574 CASREACT
 T1 Polytriazoles as Copper(I)-Stabilizing Ligands in Catalysis
 AU Chan, Timothy R.; Hlgraf, Robert; Sharpless, K. Barry; Fokin, Valery V.
 CS Department of Chemistry and the Skaggs Institute for Chemical Biology,
 Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Organic Letters (2004), 6(17), 2853-2855
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 AB Polytriazolylamines were synthesized by the copper(I)-catalyzed
 ligation of azides and alkynes. The C3-sym. derivative, TBTA, was shown to
 be a powerful stabilizing ligand for copper(I), protecting it from
 oxidation and disproportionation, while enhancing its catalytic activity.

RX(1) OF 21 A + 3 B ==> C

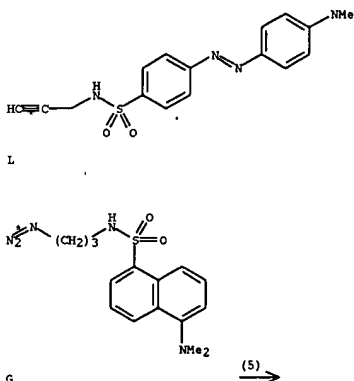


RX(1) RCT A 6921-29-5, B 72320-38-8
 RGT D 108-48-5 2,6-Lutidine
 PRO C 760952-88-3
 CAT 64443-05-6 Copper(I+), tetrakis(acetonitrile)-, (T-4)-,
 hexafluorophosphate(1-)
 SOL 75-05-8 MeCN
 RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 57 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

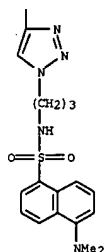
L4 ANSWER 58 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 141:242977 CASREACT
 T1 Discovery and characterization of catalysts for azide-alkyne cycloaddition
 by fluorescence quenching
 AU Lewis, Warren G.; Magallon, Fernando G.; Fokin, Valery V.; Finn, M. G.
 CS Department of Chemistry, The Scripps Research Institute, The Skaggs
 Institute for Chemical Biology, La Jolla, CA, 92037, USA
 SO Journal of the American Chemical Society (2004), 126(30), 9152-9153
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB Copper-based catalysts for the 1,3-dipolar cycloaddn. of azides
 and alkynes were screened in parallel fashion using a fluorescence
 quenching assay. The method was designed to identify systems able to
 accelerate the coupling of reactants at micromolar concns. in aqueous mixts.
 and to obtain quant. comparisons of their activities. In addition to the
 tris(triazolylamine) previously reported, two types of compds. (bipy/phen
 and 2-pyridyl Schiff bases) were found to exhibit significant
 ligand-accelerated catalysis, with one complex showing especially dramatic
 rate enhancements. Preliminary explorations of the dependence of reaction rate
 on pH, ligand:Cu ratio, and Cu concentration are described.

RX(5) OF 22 ...L + G ==> P



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L4 ANSWER 58 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
PAGE 2-A

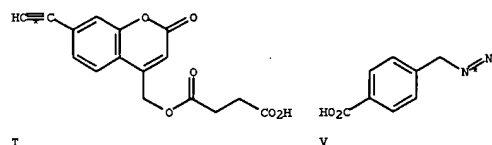


P
YIELD 81%

RX(5) RCT L 750597-28-5, G 610794-21-3
RGT Q 134-03-2 Na ascorbate
PRO P 750597-29-6
CAT 7758-98-7 CuSO4
SOL 7732-18-5 Water, 67-68-5 DMSO
CON overnight, room temperature
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

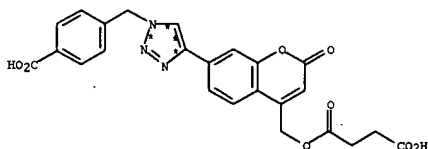
L4 ANSWER 59 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
AN 141:190399 CASREACT
TI A Fluorogenic Probe for the Copper(I)-Catalyzed Azide-Alkyne
Ligation Reaction: Modulation of the Fluorescence Emission via
3(n,π*)-1(π,π*) Inversion
AU Zhou, Zhen; Fahrni, Christoph J.
CS School of Chemistry and Biochemistry, Georgia Institute of Technology,
Atlanta, GA, 30332, USA
SO Journal of the American Chemical Society (2004), 126(29), 8862-8863
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Chemoselective ligation reactions represent a powerful approach for
labeling of proteins or small mols. in a biol. environment. We report
here a fluorogenic probe that is activated by a bio-orthogonal and
chemoselective ligation reaction which is based on the azide moiety as a
functional group. The electron-donating properties of the triazole ring
that is formed in the course of the coupling reaction were effectively
utilized to modulate the fluorescence output of the electronically coupled
coumarin fluorophore. Under physiol. conditions the probe is essentially
nonfluorescent and undergoes a bright emission enhancement upon ligation
with azide. Time-resolved emission spectroscopy and semiempirical
quantum-mech. calcs. suggest that the fluorescence switching is due to
inversion of the energy order of the emissive 1(π,π*) and
nonemissive 3(n,π*) excited states. The rapid kinetics of the ligation
reaction makes the probe attractive for a wide range of applications in
biol., anal. chemical, or material science.

RX(7) OF 33 ...T + V ==> W



(7) →

L4 ANSWER 59 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

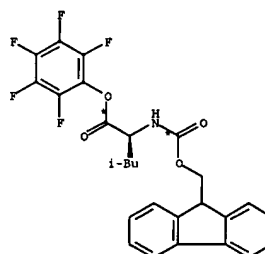


V
YIELD 76%

RX(7) RCT T 736957-98-5, V 79584-03-5
STAGE(1)
RGT X 7758-98-7 CuSO4, Y 50-81-7 (L)-Ascorbic acid
SOL 7732-18-5 Water, 75-65-0 t-BuOH
CON 2 days, room temperature
STAGE(2)
SOL 7732-18-5 Water
CON room temperature
PRO W 736957-99-6
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

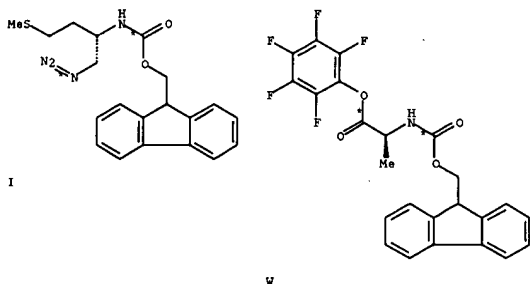
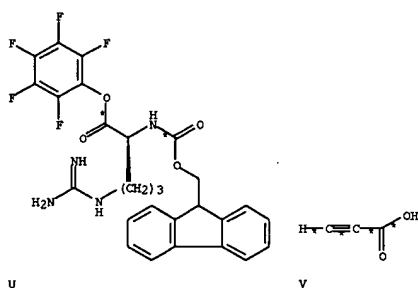
L4 ANSWER 60 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
AN 141:401 CASREACT
TI Combinatorial Library of Peptidotriazoles: Identification of
[1,2,3]-Triazole Inhibitors against a Recombinant Leishmania mexicana
Cysteine Protease
AU Tornøe, Christian W.; Sanderson, Sanya J.; Mottram, Jeremy C.; Coombs,
Graham H.; Meldal, Morten
CS Center for Solid-Phase Organic Combinatorial Chemistry, Department of
Chemistry, Carlsberg Laboratory, Valby, DK-2500, Den.
SO Journal of Combinatorial Chemistry (2004), 6(3), 312-324
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
AB A library consisting of about half of 800 000 possible peptidotriazoles on
450 000 beads was prepared by solid-phase peptide synthesis combined with a
regiospecific copper(I)-catalyzed 1,3-dipolar cycloaddn. between a
resin-bound alkyne and a protected amino azide. The central
[1,2,3]-triazole was flanked on each side by two randomized amino acids
introduced in a combinatorial approach. Importantly, the formation of the
triazole could be performed quant. in a randomized fashion. The library
was screened on solid phase for inhibitory effect against a recombinant
cysteine protease, Leishmania mexicana CPB2.8ACTE and sorted by a
high-throughput instrument, COPAS beadsorter (up to 200 000 beads/h).
Forty-eight hits were analyzed by MALDI-TOF MS providing structural
information about the protease specificity, and 23 peptidotriazoles were
resynthesized and evaluated in solution, with the best inhibitor displaying
a
Ki value of 76 nM. A one-pot procedure was used to convert Fmoc-amino
azides into their corresponding Boc derivs. The crucial influence of weak
interactions with a spacer used for detection by MALDI-TOF MS on screening
results was observed

RX(6) OF 28 T + U + V + I + W + X ==> Y



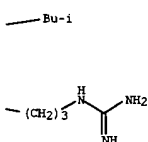
T

L4 ANSWER 60 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L4 ANSWER 60 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



Y
YIELD 57%

RX (6)

```

STAGE(1)
  RGT  Z 125700-67-6 Benzotriazolium der, AA 100-74-3
      4-Ethylmorpholine

STAGE(2)
  RGT  D 110-89-4 Piperidine
  SOL  68-12-2 DMF

STAGE(3)
  RCT  T 85060-88-0
  RGT  Z 125700-67-6 Benzotriazolium der, AB 28230-32-2
      Benzotriazinolone

STAGE(4)
  RGT  D 110-89-4 Piperidine
  SOL  68-12-2 DMF

STAGE(5)
  RCT  U 135793-01-0
  RGT  Z 125700-67-6 Benzotriazolium der, AB 28230-32-2
      Benzotriazinolone

STAGE(6)
  RGT  D 110-89-4 Piperidine
  SOL  68-12-2 DMF

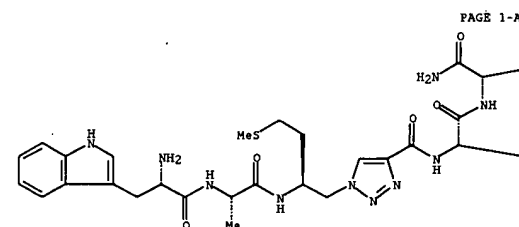
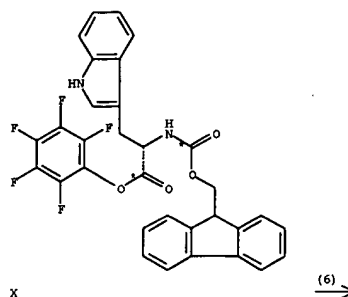
STAGE(7)
  RCT  V 471-25-0
  RGT  AC 16357-59-8 EEDQ

STAGE(8)
  RCT  I 432507-63-6
  CAT  7681-65-4 CuI
  SOL  110-86-1 Pyridine

STAGE(9)
  RGT  D 110-89-4 Piperidine
  SOL  68-12-2 DMF

```

L4 ANSWER 60 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L4 ANSWER 60 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

```

STAGE(10)
  RCT   W 86060-86-8
  RGT   Z 125700-67-6 Benzotriazolium der, AB 28230-32-2
        Benzotriazinolone

STAGE(11)
  RGT   D 110-89-4 Piperidine
  SOL   68-12-2 DMF

STAGE(12)
  RCT   X 86069-87-6
  RGT   Z 125700-67-6 Benzotriazolium der, AB 28230-32-2
        Benzotriazinolone

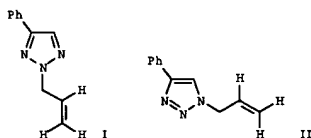
STAGE(13)
  RGT   D 110-89-4 Piperidine
  SOL   68-12-2 DMF

STAGE(14)
  RGT   AD 13154-24-0 (i-Pr)3SiCl, AE 76-05-1 F3CCO2H
  SOL   7732-18-5 Water
  CON   SUBSTAGE(1) . 5 hours, room temperature
        SUBSTAGE(2) . 5 hours, room temperature
        SUBSTAGE(3) . 5 hours, room temperature
        SUBSTAGE(4) . 5 hours, room temperature
        SUBSTAGE(5) . 5 hours, room temperature

```

PRO Y 693784-62-2
NTE solid-supported reaction, first stage derivatization of PEGA800
resin with Rink amide linker, third stage attachment to
solid-state resin
99 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 61 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 140:339262 CASREACT
 TI A one-pot procedure for the regiocontrolled synthesis of allyltriazoles
 via the Pd-Cu bimetallic-catalyzed three-component coupling reaction of
 nonactivated terminal alkynes, allyl carbonate, and trimethylsilyl azide
 AU Kamiyo, Shin; Jin, Tienan; Huo, Zhibao; Yamamoto, Yoshinori
 CS Research Center for Sustainable Materials Engineering, Institute of
 Multidisciplinary Research for Advanced Materials, and Department of
 Chemistry, Graduate School of Science, Tohoku University, Sendai,
 980-8578, Japan
 SO Journal of Organic Chemistry (2004), 69(7), 2386-2393
 CODEN: JOCEHH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 GI



AB A one-pot procedure for the regiocontrolled synthesis of both 2-allyl- and 1-allyl-1,2,3-triazoles by the three-component coupling reaction of nonactivated terminal alkynes with allyl carbonate and trimethylsilyl azide, under palladium and copper bimetallic catalyst, has been developed. To accomplish the regioselective synthesis of the allyltriazoles, proper choice of two different catalyst systems was needed. The combination of Pd2(dba)3·CHCl3-CuCl(PPh3)3-P(OPh)3 catalyzed the formation of 2-allyl-1,2,3-triazoles, e.g., I, while the combination of Pd(OAc)2-CuBr2-PPh3 promoted the formation of 1-allyl-1,2,3-triazoles, e.g., II. The cooperative activity of palladium and copper catalysts played an important role in the presented transformations. Most probably, the palladium catalyst worked as a catalyst for generating reactive azide species, π -allylpalladium azide complex and allyl azide. The copper catalyst probably activated the C-C triple bond of the starting terminal alkynes by forming a copper-acetylide intermediate and thereby promoted the [3 + 2]-cycloaddn. reaction between the reactive azide species and the copper-acetylide to form the triazole framework.

RX(3) OF 22 H + A ==> D

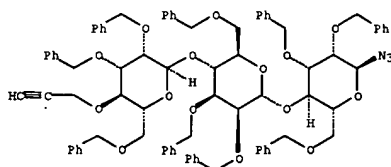
L4 ANSWER 61 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

Ph-CH=CH
 H
 A
 (3)
 D
 YIELD 88%

RX(3) RCT H 536-74-3, A 35466-83-2
 RGT I 4648-54-8 Me3SiN3
 PRO D 679842-59-2
 CAT 3375-31-3 Pd(OAc)2, 7789-45-9 CuBr2, 603-35-0 PPh3
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 3 hours, 80 deg C
 NTE regioselective, optimized on catalyst system and solvent, yield and regioselectivity depend on catalyst system and solvent
 RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 62 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 140:287594 CASREACT
 TI Synthesis of Readily Modifiable Cyclodextrin Analogues via
 Cyclodimerization of an Alkynyl-Azido Trisaccharide
 AU Bodine, Kyle D.; Gin, David Y.; Gin, Mary S.
 CS Department of Chemistry, University of Illinois at Urbana-Champaign,
 Urbana, IL, 61801, USA
 SO Journal of the American Chemical Society (2004), 126(6), 1638-1639
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB A convergent strategy for the synthesis of β -cyclodextrin analogs is reported, utilizing preferential cyclodimerization of an azido-alkyne trisaccharide via Cu(I)-catalyzed [3+2] dipolar cycloaddn. of the alkyne and azide functional groups. The resultant oligosaccharide macrocycle retains the binding propensity of cyclodextrins, as demonstrated by the similar 8-anilino-1-naphthalenesulfonate (ANS) association consts. This new synthetic strategy opens up new avenues for modular preparation of functionally diverse cyclodextrin analogs that are otherwise inaccessible.

RX(11) OF 114 ...AA ==> AC + AD...



AA



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

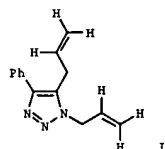
L4 ANSWER 62 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STRUCTURE
 DIAGRAM
 IS NOT
 AVAILABLE

AD
 YIELD 15%

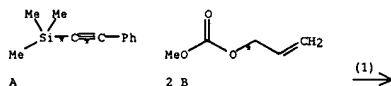
RX(11) RCT AA 674777-82-3
 RGT AE 6674-22-2 DBU
 PRO AC 674777-83-4, AD 675623-08-2
 CAT 7681-65-4 CuI
 SOL 108-88-3 PhMe
 CON 16 hours, 50 deg C
 NTE other product also detected
 RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 63 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 140:217574 CASREACT
 TI Four-component coupling reactions of silylacetylenes, allyl carbonates, and trimethylsilyl azide catalyzed by a Pd(0)-Cu(I) bimetallic catalyst. Fully substituted triazole synthesis from seemingly internal alkynes
 AU Kamiyo, Shin; Jin, Tienan; Yamamoto, Yoshinori
 CS Institute of Multidisciplinary Research for Advanced Materials, Research Center for Sustainable Materials Engineering, Tohoku University, Sendai, 980-8578, Japan
 SO Tetrahedron Letters (2004), 45(4), 689-691
 CODEN: TETL; ISSN: 0040-4039
 PB Elsevier Science B.V.
 DT Journal
 LA English
 GI



AB Fully substituted triazoles, e.g., I, were synthesized by the four-component coupling reaction of unactivated silylacetylenes, two equivalent of allyl carbonates, and trimethylsilyl azide, in the presence of a Pd(0)-Cu(I) bimetallic catalyst. The trisubstituted 1,2,3-triazoles were obtained in good yields. The reaction most probably proceeds through the [3 + 2]-cycloaddn. reaction between the alkynylcopper species and azide followed by the cross-coupling reaction between the vinylcopper intermediate and π -allylpalladium complex.

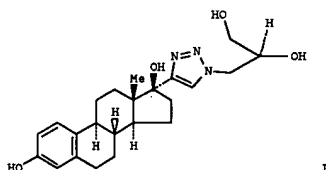
RX(1) OF 19 A + 2 B ==> C



APPLICANT

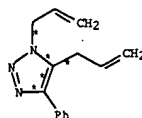
L4 ANSWER 64 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 140:27830 CASREACT
 TI Process for preparation of 1,4-disubstituted [1,2,3]-triazoles by metal-catalyzed, in particular copper-catalyzed, regioselective Huisgen 1,3-dipolar cycloaddition of azides and acetylenes
 IN Sharpless, K. Barry; Fokin, Valery; Rostovsev, Vsevolod; Green, Luke; Himo, Fahmi
 PA The Scripps Research Institute, USA
 SO PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003101972	A1	20031211	WO 2003-US17311	20030530
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZH, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2487424	A1	20031211	CA 2003-2487424	20030530
AU 2003240482	A1	20031219	AU 2003-240482	20030530
EP 1507769	A1	20050223	EP 2003-731490	20030530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671673	A	20050921	CN 2003-817917	20030530
JP 200602099	T	20060119	JP 2004-509665	20030530
US 2005222427	A1	20051006	US 2005-516671	20050516
PRAI US 2002-385041P		20020530		
WO 2003-US17311		20030530		



AB The invention is directed to a process for Huisgen 1,3-dipolar cycloaddn. of azides and terminal acetylenes for forming 1,4-disubstituted [1,2,3]-triazoles regioselectively, catalyzed by the addition of Cu(II) in the presence of a reducing agent, for reducing Cu(II) to Cu(I), in situ, in catalytic amount. The invention also discloses the use of aqueous Cu(I) salts, and other metals such as Au, Ag, Hg, Cd, Pt and Pd. The advantages include lower reaction temps., even room temperature, high regioselectivity, use

L4 ANSWER 63 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

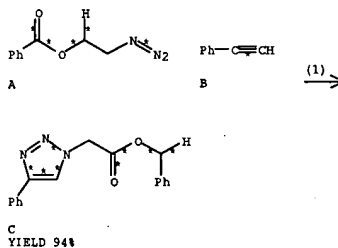


C
 YIELD 77%

RX(1) RCT A 2170-06-1, B 35466-83-2
 RGT D 4648-54-8 Me3SiN3
 PRO C 665012-61-3
 CAT 51364-51-3 Ph2-pentadienone Pd, 7758-89-6 CuCl, 122-52-1 P(OEt)3
 SOL 123-91-1 Dioxane
 CON 8 hours, 100 deg C
 RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 64 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 of the cheaper and purer Cu(II) salts, and no functional group interference. For instance, I was prepd., in 94% yield, by Huisgen 1,3-dipolar cycloaddn. of 17-ethynyl estradiol and (S)-3-azidopropane-1,2-diol in the presence of 1 mol% CuSO4·5H2O and 10 mol% sodium ascorbate in water/t-BuOH mixt. at room temp. overnight.

RX(1) OF 12 A + B ==> C

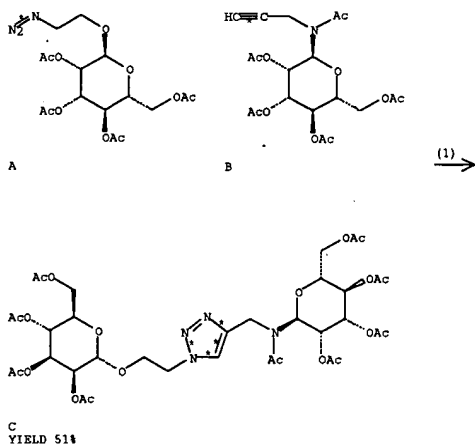


C
 YIELD 94%

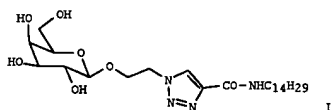
RX(1) RCT A 475599-41-8, B 536-74-3
 RGT D 134-03-2 Na ascorbate
 PRO C 478555-22-5
 CAT 7758-89-6 CuSO4·5H2O
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 12 - 24 hours, room temperature
 RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 65 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 139:85565 CASREACT
 TI Multivalent Neoglycoconjugates by Regiospecific Cycloaddition of Alkynes and Azides Using Organic-Soluble Copper Catalysts
 AU Perez-Balderas, Francisco; Ortega-Munoz, Mariano; Morales-Sanfrutos, Julia; Hernandez-Mateo, Fernando; Calvo-Flora, Francisco G.; Calvo-Asin, Jose A.; Isac-Garcia, Joaquin; Santoyo-Gonzalez, Francisco
 CS Instituto de Biotecnologia Facultad de Ciencias, Universidad de Granada, Granada, E-18071, Spain
 SO Organic Letters (2003), 5(11), 1951-1954
 CODEN: ORLEF7; ISSN: 1523-7060
 DT Journal
 LA English
 AB The construction of multivalent neoglycoconjugates is efficiently achieved by the regiospecific catalytic cycloaddn. of alkynes and azides using the organic-soluble copper complexes (Ph₃P)₃CuBr and (EtO)₃P·CuI. The simultaneous use of microwave irradiation shortened notably the reaction times.

RX(1) OF 23 ...A + B ==> C

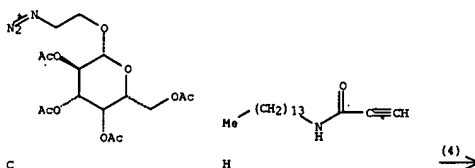


L4 ANSWER 66 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 138:90001 CASREACT
 TI Synthesis of Sugar Arrays in Microtiter Plate
 AU Fazio, Fabio; Bryan, Marian C.; Blixt, Olaf; Paulson, James C.; Wong, Chi-Huey
 CS Department of Chemistry and Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Journal of the American Chemical Society (2002), 124(48), 14397-14402
 CODEN: JACSAT; ISSN: 0002-7863
 DT Journal
 LA English
 GI



AB 1,3-Dipolar cycloaddns. between azides and alkynes were exploited to attach oligosaccharides to a C14 hydrocarbon chain that non-covalently binds to the microtiter well surface. Synthesis of sugar arrays was performed on a micromolar scale in situ in the microtiter plate. As a model study, the β -galactosyllipid I was displayed on a 4- μ mol scale. Formation of product was confirmed via ESI-MS, and the yield was determined via chemical and biol. assays. Several complex carbohydrates were also displayed in microtiter plates and successfully screened with various lectins. Moreover, sialyl Lewis x was synthesized via the enzymic fucosylation of a precursor displayed in the plate. Studies on inhibition of this biotransformation have been carried out.

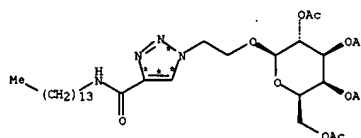
RX(4) OF 21 ...C + H ==> N



L4 ANSWER 65 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(1) RCT A 140428-83-7, B 548464-03-5
 RGT D 6674-22-2 DBU
 PRO C 548464-12-6
 CAT 15709-74-7 Copper, bromotris(triphenylphosphine)-, (T-4)-
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) 2 minutes
 SUBSTAGE(2) 45 minutes
 NTE microwave irradiatn.
 RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

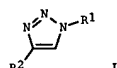
L4 ANSWER 66 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 89%

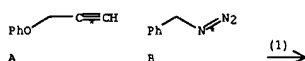
RX(4) RCT C 139888-80-5, H 146722-52-3
 PRO N 482617-94-7
 SOL 67-56-1 MeOH
 CON 24 hours, 80 deg C
 RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 67 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 138:39236 CASREACT
 TI A stepwise Huisgen cycloaddition process: copper(I)-catalyzed regioselective "ligation" of azides and terminal alkynes
 AU Rostovtsev, Vsevolod V.; Green, Luke G.; Fokin, Valery V.; Sharpless, K. Barry
 CS Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Angewandte Chemie, International Edition (2002), 41(14), 2596-2599
 CODEN: ACIEF5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH
 DT Journal
 LA English
 GI



AB 1,4-Disubstituted 1,2,3-triazoles I (R1 = PhCH2, PhCH2OCH2, 1-adamantyl, etc.; R2 = HO2C, Ph, PhOCH2, Et2NCH2, etc.) were readily and cleanly prepared via highly efficient and regioselective copper (I)-catalyzed cycloaddn. of azides R1N3 with terminal alkynes R2C.tpbond.CH in 82-93% yields.

RX(1) OF 13 A + B ==> C



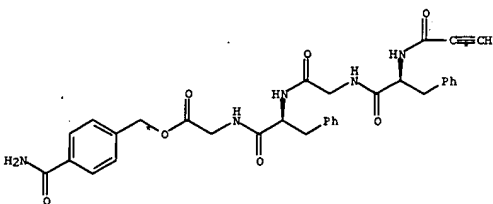
C
 YIELD 91%

RX(1) RCT A 13610-02-1, B 622-79-7

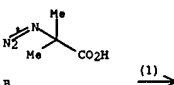
STAGE(1)
 RGT D 134-03-2 Na ascorbate, E 7758-99-8 CuSO4.5H2O
 SOL 7732-18-5 Water, 75-65-0 t-BuOH
 CON 8 hours, room temperature

L4 ANSWER 68 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 137:6388 CASREACT
 TI Peptidotriazoles on Solid Phase: [1,2,3]-Triazoles by Regioselective Copper(I)-Catalyzed 1,3-Dipolar Cycloadditions of Terminal Alkynes to Azides
 AU Tornøe, Christian W.; Christensen, Caspar; Meldal, Morten
 CS Center for Solid Phase Organic Combinatorial Chemistry Department of Chemistry, Carlsberg Laboratory, Valby, DK-2500, Den.
 SO Journal of Organic Chemistry (2002), 67(9), 3057-3064
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 AB The cycloaddn. of azides to alkynes is one of the most important synthetic routes to 1H-[1,2,3]-triazoles. This work reports a novel regioselective copper(I)-catalyzed 1,3-dipolar cycloaddn. of terminal alkynes to azides on solid-phase. Primary, secondary, and tertiary alkyl azides, aryl azides, and an azido sugar were used successfully in the copper(I)-catalyzed cycloaddn. producing diversely 1,4-substituted [1,2,3]-triazoles in peptide backbones or side chains. The reaction conditions were fully compatible with solid-phase peptide synthesis on polar supports. The copper(I) catalysis is mild and efficient (>95% conversion and purity in most cases) and furthermore, the x-ray structure of 2-azido-2-methylpropanoic acid has been solved, to yield structural information on the 1,3-dipoles entering the reaction. Novel Fmoc-protected amino azides were prepared from Fmoc-amino acids by Mitsunobu reaction.

RX(1) OF 6 A + B ==> C



A
 resin-bound



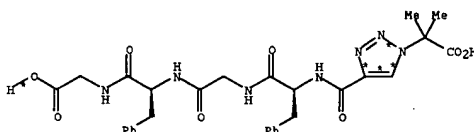
B

L4 ANSWER 67 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)
 SOL 7732-18-5 Water

PRO C 478555-18-9
 RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 68 OF 69 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

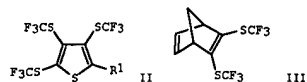
RX(1) RCT A 432507-18-1D, B 2654-97-9

STAGE(1)
 RGT D 7087-68-5 EtN(Pr-i)2
 CAT 7681-65-4 CuI
 SOL 109-99-9 THF

STAGE(2)
 RGT E 1310-73-2 NaOH
 SOL 7732-18-5 Water

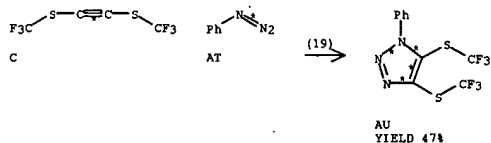
PRO C 432507-19-2
 NTE first stage solid-supported and regioselective; >95% conversion
 RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 69 OF 69 CASREACT COPYRIGHT 2006 ACS on STN
 AN 109:230224 CASREACT
 TI Syntheses and reactions of trifluoromethylchalcogen derivatives of alkynes
 AU Haas, Alois; Kraechter, Hans Udo
 CS Ruhr-Univ., Bochum, D-4630/1, Fed. Rep. Ger.
 SO Chemische Berichte (1988), 121(10), 1833-40
 CODEN: CHBEAM; ISSN: 0009-2940
 DT Journal
 LA German
 GI



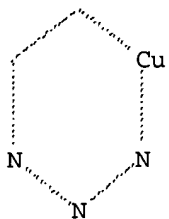
AB RC.tplbond.CXCF3 (R = Ph, F3CSCH2, X = S, R = H, X = CH2S, CH2Se) were prepared by treating bromoalkynes with CuSCF3 or CuSeCF3. F3CSC.tplbond.CSCF3 (I) was obtained by bromination of F3CSCH:CHSCF3 followed by elimination of HBr. Reactions of I were investigated. Thus, photolysis of I gave thiophenes II (R1 = CF3, SCF3). I underwent cycloaddn. with cyclopentadiene to given adduct III.

RX(19) OF 68 ...C + AT ==> AU



RX(19) RCT C 2069-87-6, AT 622-37-7
 PRO AU 114861-76-6

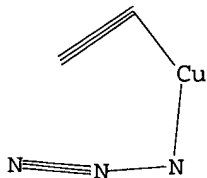
=> => d que 17 stat
L5 STR



Structure attributes must be viewed using STN Express query preparation.
L7 0 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 1067 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

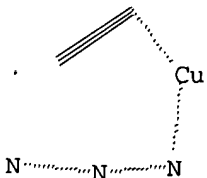
=> => d que 110 stat
L8 STR



Structure attributes must be viewed using STN Express query preparation.
L10 0 SEA FILE=REGISTRY SSS FUL L8

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

=> => d que 111 stat
L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> => d que 123 stat
L14 389 SEA FILE=CAPLUS ABB=ON PLU=ON "SHARPLESS K BARRY"/AU

L15 76 SEA FILE=CAPLUS ABB=ON PLU=ON ("FOKIN VALERY"/AU OR "FOKIN
 VALERY V"/AU)
L16 17 SEA FILE=CAPLUS ABB=ON PLU=ON ("ROSTOVTSEV VSEVOLOD"/AU OR
 "ROSTOVTSEV VSEVOLOD V"/AU OR "ROSTOVTSEV VSEVOLOD VLADIMIROVIC
 H"/AU)
L17 17 SEA FILE=CAPLUS ABB=ON PLU=ON ("GREEN LUKE"/AU OR "GREEN
 LUKE G"/AU OR "GREEN LUKE GIDEON GRANVILLE"/AU OR "GREEN LUKE
 M"/AU)
L18 48 SEA FILE=CAPLUS ABB=ON PLU=ON "HIMO FAHMI"/AU
L19 489 SEA FILE=CAPLUS ABB=ON PLU=ON L14 OR L15 OR L16 OR L17 OR
 L18
L20 41 SEA FILE=CAPLUS ABB=ON PLU=ON L19 AND TRIAZOLE
L21 39 SEA FILE=CAPLUS ABB=ON PLU=ON L20 AND AZIDE
L22 36 SEA FILE=CAPLUS ABB=ON PLU=ON L21 AND (ACETYLENE OR ALKYNE)
L23 24 SEA FILE=CAPLUS ABB=ON PLU=ON L22 AND COPPER

=> d 1-24 bib abs

L23 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2006:1250367 CAPLUS
 TI Rapid Discovery and Structure-Activity Profiling of Novel Inhibitors of Human Immunodeficiency Virus Type 1 Protease Enabled by the Copper (I)-Catalyzed Synthesis of 1,2,3-Triazoles and Their Further Functionalization
 AU Whiting, Matthew; Tripp, Jonathan C.; Lin, Ying-Chuan; Lindstrom, William Olson, Arthur J.; Elder, John H.; Sharpless, K. Barry; Fokin, Valery V.
 CS Departments of Chemistry and Molecular Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Journal of Medicinal Chemistry ACS ASAP
 CODEN: JMCMAH; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 AB Building from the results of a computational screen of a range of triazole-containing compds. for binding efficiency to human immunodeficiency virus type 1 protease (HIV-1-Pr), a novel series of potent inhibitors has been developed. The copper(I)-catalyzed azide-alkyne cycloaddn. (CuAAC), which provides ready access to 1,4-disubstituted 1,2,3-triazoles, was used to unite a focused library of azide-containing fragments with a diverse array of functionalized alkyne-containing building blocks. In combination with direct screening of the crude reaction products, this method led to the rapid identification of a lead structure and readily enabled optimization of both azide and alkyne fragments. Replacement of the triazole with a range of alternative linkers led to greatly reduced protease inhibition; however, further functionalization of the triazoles at the 5-position gave a series of compds. with increased activity, exhibiting K_i values as low as 8 nM.
 RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2006:862506 CAPLUS
 TI Ruthenium-catalyzed dipolar cycloaddition of organic azides and alkynes
 AU Boren, Brant; Narayan, Sridhar; Rasmussen, Lars K.; Jia, Guochen; Fokin, Valery V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Abstracts of Papers, 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006 (2006), ORGN-365 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69IHRO
 DT Conference/ Meeting Abstracts (computer optical disk)
 LA English
 AB Ru(II) complexes, such as $\text{Cp}^*\text{RuCl}(\text{PPh}_3)_2$, regioselectively catalyze 1,3-dipolar cycloaddn. of organic azides and alkynes. Diversely functionalized 1,5-disubstituted triazoles are usually obtained in good to excellent yield after heating the reaction mixture at 50 - 80 °C for several hours. Furthermore, internal alkynes also participate in the catalysis, producing 1,4,5-trisubstituted 1,2,3-triazoles. Thus, the ruthenium system complements the copper-catalyzed azide-alkyne cycloaddn., providing facile access to wide range of 1,2,3-triazoles with different substitution patterns.

L23 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2006:860801 CAPLUS
 TI Catalytic dipolar cycloaddition of azides and alkynes: The reach of one reaction
 AU Fokin, Valery V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Abstracts of Papers, 232nd ACS National Meeting, San Francisco, CA, United States, Sept. 10-14, 2006 (2006), INOR-409 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69IHRO
 DT Conference/ Meeting Abstracts (computer optical disk)
 LA English
 AB Despite the high energy content, organic azides are chemical inert to an unusually broad range of reagents, solvents, and functional groups. This orthogonality allows them to remain "invisible" through most synthetic (and biosynthetic) steps without the need for protecting groups. The special reactivity of azides can be revealed in the dipolar cycloaddn. with alkynes, which produces 1,2,3-triazoles. However, the high energy of activation (ca. 24-26 kcal/mol) makes the thermal cycloaddn. very slow and inefficient even at elevated temperature. Copper(I) catalysts accelerate the reaction by seven to eight orders of magnitude, resulting in regioselective formation of 1,4-disubstituted 1,2,3-triazoles. This catalytic "fusion" of azides and terminal alkynes exhibits remarkable fidelity and has been shown to perform well even in complex biol. systems. Addnl., ruthenium(II) has recently joined the repertoire of catalysts, providing ready access to the complementary 1,5-regioisomers as well as fully substituted triazoles. The presentation will compare the two catalytic processes, addressing their key practical aspects and current limitations, and will highlight their representative applications.

L23 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2006:496447 CAPLUS
 DN 145:27683
 TI Practical synthesis of amides from in situ generated copper(I) acetylides and sulfonyl azides
 AU Cassidy, Michael P.; Raushel, Jessica; Fokin, Valery V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Angewandte Chemie, International Edition (2006), 45(19), 3154-3157
 CODEN: ACHIEF; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 AB A direct, simple, and efficient route from terminal alkynes to amides is achieved by their copper(I)-catalyzed reaction with sulfonyl azides. The reaction proceeds with the in situ generation of copper(I) acetylides and represents a one-step formal oxidative hydration of a triple bond.
 RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2006:101293 CAPLUS
DN 144:192955
TI Polymeric materials via click chemistry
IN Fokin, Valery; Finn, M. G.; Sharpless, K. Barry
PA The Scripps Research Institute, USA
SO PCT Int. Appl., 59 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006012569	A1	20060202	WO 2005-US26177	20050722
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRAI US 2004-590885P P 20040722

AB Adhesive polymers are formed when polyvalent azides and polyvalent alkynes are assembled into crosslinked polymer networks by copper-catalyzed 1,3-dipolar cycloaddn. The condensation polymerization is efficiently promoted by Cu ions either leached

from the metal surface or added to the monomer mixture, and strong interactions with metal surfaces are provided by the multiple triazole binding elements produced. The adhesive polymers may be formed either as adhesive polymer coatings or as adhesive polymer cement. A typical adhesive for bonding Cu plates was based on THF containing 2,2-bis(azidomethyl)-1,3-propanediol and N(CH₂C.tplbond.CH)₃ in a N3-C.tplbond.CH mol ratio 1:1.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2006:29374 CAPLUS
DN 144:108794
TI Click chemistry route to triazole diverse dendrimers by copper(I)-catalyzed ligation of azides and alkynes
IN Fokin, Valery; Sharpless, K. Barry; Wu, Peng; Feldman, Alina
PA The Scripps Research Institute, USA
SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006005046	A2	20060112	WO 2005-US23718	20050630
WO 2006005046	A9	20060309		
WO 2006005046	A3	20061130		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI US 2004-584817P P 20040630

OS MARPAT 144:108794

AB The high efficiency and fidelity of click chemical permits a large number of diverse dendrimers encompassing a wide variety of functionalities at the chain ends, repeat units, and/or core to be prepared. Almost quant. yields were obtained during the synthesis. In some cases, filtration or solvent extraction was the only method required for purification. These features represent a

significant advancement in dendrimer chemical and demonstrate an evolving synergy between organic chemical and functional materials.

L23 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1225912 CAPLUS
DN 144:107989
TI NH-1,2,3-triazoles from azidomethyl pivalate and carbamates: Base-labile N-protecting groups
AU Loren, Jon C.; Krasinski, Antoni; Fokin, Valery V.; Sharpless, K. Barry
CS The Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Synlett (2005), (18), 2847-2850
CODEN: SYNLES; ISSN: 0936-5214
PB Georg Thieme Verlag
DT Journal
LA English
OS CASREACT 144:107989

AB Protected 1,2,3-triazoles are prepared by copper-catalyzed dipolar cycloaddn. reactions of acyloxymethyl azides RCOOCH₂N₃ (R = Me₃C, 4-morpholinyl, Et₂N) and terminal alkynes; the products are readily deprotected with aqueous sodium hydroxide followed

by neutralization to yield 1,2,3-triazoles, with the ease of deprotection dependent upon the protecting group chosen. Pivaloyloxymethyl azide is prepared by reaction of chloromethyl pivalate with sodium azide, while 4-(azidomethoxycarbonyl)morpholine and diethylcarbamoyloxymethyl azide are prepared by addition of morpholine or diethylamine to chloromethyl chloroformate followed by reaction of the chloromethyl carbamates with sodium azide; the azides are easily prepared on 0.1-mol scale. The acyl groups determine the rate of deprotection of

the protected triazoles; N-(pivaloyloxymethyl)triazoles are cleaved to 1,2,3-triazoles by treatment with aqueous sodium hydroxide for 30 min. at room temperature, while the corresponding (morpholinylcarbamoyloxymethyl)triazoles require 24 h at ambient temperature for cleavage, and the (diethylcarbamoyloxymethyl)triazoles require 24 h at 85° for cleavage. The acyloxymethyl azides are potential synthetic equivalent for hydrazoic acid in copper-catalyzed 1,3-dipolar cycloaddns.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:511289 CAPLUS
DN 143:193958
TI Kinetic resolution by copper-catalyzed azide-alkyne cycloaddition
AU Meng, Jun-cai; Fokin, Valery V.; Finn, M. G.
CS Department of Chemistry, Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
SO Tetrahedron Letters (2005), 46(27), 4543-4546
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 143:193958

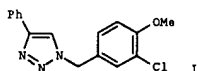
AB The use of chiral pybox ligands imparts enantioselectivity to the CuI-catalyzed azide-alkyne cycloaddn. reaction, in the form of kinetic resolution of α-chiral azides and desymmetrization of gem-diazides. While levels of selectivity are modest, the results show unequivocally that the process benefits from ligand-accelerated catalysis. Some copper complexes are known to involve a copper(I)-acetylide species; a selection of pybox ligands was screened in the kinetic resolution of a racemic azides. Each showed an acceleration rate with respect to the reaction in the absence of a chelating ligand. It was shown that the ligands are involved in the copper-catalyzed process (ligand-accelerated catalysis). The cycloaddn. of 2-[1-(azido)ethyl]naphthalene with (ethynyl)benzene gave 1-[1-(2-naphthalenyl)ethyl]-4-phenyl-1,2,3-triazole.

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:371895 CAPLUS
 DN 143:26152
 TI Mechanism of the ligand-free CuI-catalyzed azide-alkyne
 cycloaddition reaction
 AU Rodionov, Valentin O.; Fokin, Valery V.; Finn, M. G.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
 92037, USA
 SO Angewandte Chemie, International Edition (2005), 44(15), 2210-2215
 CODEN: ACIEF5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 OS CASREACT 143:26152
 AB The Cu-catalyzed azide-alkyne cycloaddn. depends on
 rapid formation of CuI-acetylide complexes from terminal alkynes
 and their ability to activate organic azides. A kinetics study
 uncovered a bimol. dependence on the metal and an unusually fast intramol.
 variant of the process.
 RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:192094 CAPLUS
 TI Asymmetric dendrimers via copper(I)-catalyzed triazole
 formation
 AU Wu, Feng; Malkoch, Michael; Hunt, Jasmine; Fokin, Valery V.;
 Sharpless, K. Barry; Hawker, Craig J.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
 92037, USA
 SO Abstracts of Papers, 229th ACS National Meeting, San Diego, CA, United
 States, March 13-17, 2005 (2005), ORGN-070 Publisher: American Chemical
 Society, Washington, D. C.
 CODEN: 69GQMP
 DT Conference; Meeting Abstract
 LA English
 AB The mild reaction conditions and high efficiency of copper
 (I)-catalyzed dipolar cycloaddn. of azides and alkynes
 are exploited in the synthesis of a series of amphiphilic, diblock
 dendrimers, in which the number of chain ends in each dendritic block is
 easily controlled. The unique asym. character of the dendrimers combined
 with the unprecedented functional group compatibility of the cycloaddn.
 permits sequential derivatizations of the periphery to introduce a variety
 of functionalities, such as biol. active moieties and reporter tags. The
 chemical and phys. properties, as well as the potential applications of the
 resulting macromols. will be addressed.

L23 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:870376 CAPLUS
 DN 142:56242
 TI A microwave-assisted click chemistry synthesis of 1,4-disubstituted 1,2,3-
 triazoles via a copper(I)-catalyzed three-component
 reaction
 AU Appukkuttan, Prasad; Dehaen, Wim; Fokin, Valery V.; Van der
 Eycken, Erik
 CS Department of Chemistry, University of Leuven, Louvain, B-3001, Belg.
 SO Organic Letters (2004), 6(23), 4223-4225
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 142:56242
 GI



AB A microwave-assisted three-component reaction was used to prepare a series
 of 1,4-disubstituted-1,2,3-triazoles, e.g., **1**, from
 corresponding alkyl halides, sodium azide, and alkynes
 . This procedure eliminated the need to handle organic azides, as
 they were generated in situ, making this already powerful click process
 even more user-friendly and safe.
 RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:658983 CAPLUS
 TI Synthesis and biological evaluation of [1,2,3]-triazole
 vancomycin derivatives
 AU Silverman, Steven M.; Sharpless, K. Barry; Fokin, Valery
 V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
 92037, USA
 SO Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United
 States, August 22-26, 2004 (2004), ORGN-721 Publisher: American Chemical
 Society, Washington, D. C.
 CODEN: 69PTZ8
 DT Conference; Meeting Abstract
 LA English
 AB Growing resistance to known antibiotics is a cause of apprehension amongst
 public health officials. Vancomycin figures prominently in the quest to
 counter these bacteria, but strains resistant even to this glycopeptide
 antibiotic of last resort have emerged. Promising approaches to
 increasing the antibacterial activity of vancomycin include modification
 of the periphery and polyvalency. While numerous such semisynthetic
 deriva. of vancomycin have been prepared and evaluated, many of the methods
 used in the synthesis of these compds. involve harsh conditions, tedious
 purifications, and result in low yields. Click chemical provides a novel
 solution to these problems. Recent developments in our laboratory have
 provided a
 reliable and rapid route to 1,4-disubstituted [1,2,3]-triazoles
 via a copper(I)-catalyzed ligation of azides and
 terminal alkynes. Here we report the application of this
 methodol. towards the synthesis of a series of vancomycin homo- and
 heterodimers. The reaction was markedly successful, despite the diverse
 array of functionality present in vancomycin. The improved biol.
 activity, ease of preparation, and scalability of these reactions make these
 compds. suitable candidates for further clin. studies.

L23 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:650825 CAPLUS
 DN 141:314727
 TI Efficiency and fidelity in a click-chemistry route to triazole dendrimers by the copper(I)-catalyzed ligation of azides and alkynes
 AU Wu, Peng; Feldman, Alina K.; Nugent, Anne K.; Hawker, Craig J.; Scheel, Arnulf; Voit, Brigitte; Pyun, Jeffrey; Frechet, Jean M. J.; Sharpless, K. Barry; Fokin, Valery V.
 CS IBM Almaden Research Center, San Jose, CA, 95120, USA
 SO Angewandte Chemie, International Edition (2004), 43(30), 3928-3932
 CODEN: ACIEF5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 OS CASREACT 141:314727
 AB A large number of diverse dendrimers was prepared with high purity in almost quant. yield by the click-chemical transformation in copper (I)-catalyzed synthesis of 1,2,3-triazoles from azides and alkynes. In some cases filtration or solvent extraction was the only method required for purification in the highly efficient construction of the triazole units of the dendrimers. Frechet's convergent approach was utilized in dendrimer synthesis; thus, the individual branches or dendron were built sequentially, starting on the outside of the mol., and they were then coupled to a multivalent centerpiece (core) in the last step.
 RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:607094 CAPLUS
 DN 141:277574
 TI Polytriazoles as Copper(I)-Stabilizing Ligands in Catalysis
 AU Chan, Timothy R.; Hilgraf, Robert; Sharpless, K. Barry; Fokin, Valery V.
 CS Department of Chemistry and the Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Organic Letters (2004), 6(17), 2853-2855
 CODEN: ORLEP7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 141:277574
 AB Polytriazolylamines were synthesized by the copper(I)-catalyzed ligation of azides and alkynes. The C3-sym. derivative, TBTA, was shown to be a powerful stabilizing ligand for copper (I), protecting it from oxidation and disproportionation, while enhancing its catalytic activity.
 RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:234539 CAPLUS
 DN 141:24663
 TI Click chemistry in polymer synthesis
 AU Punna, Sreenivas; Diaz, David D.; Li, Chunmei; Sharpless, K. Barry; Fokin, Valery V.; Finn, M. G.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2004), 45(1), 778-779
 CODEN: ACPPAY; ISSN: 0032-3934
 PB American Chemical Society, Division of Polymer Chemistry
 DT Journal (computer optical disk)
 LA English
 AB The copper-catalyzed azide-alkyne cycloaddn. reaction has been applied to the preparation of new functional polymeric materials. This method is broadly tolerant of functional groups and extremely easy to perform. Characteristic properties of resulting poly(triazoles) and preliminary investigations of their adhesive and template recognition properties will be discussed. Among the most important features of the process is that catalytic copper can be recruited from metallic copper surfaces, and that the poly(triazole) products have strong affinity for metal surface.
 RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:229010 CAPLUS
 TI Click chemistry in polymer synthesis
 AU Punna, Sreenivas; Diaz, David D.; Li, Chunmei; Sharpless, K. Barry; Fokin, Valery V.; Finn, M. G.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), POLY-375 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69PGKM
 DT Conference; Meeting Abstract
 LA English
 AB The copper-catalyzed azide-alkyne cycloaddn. reaction has been applied to the preparation of new functional polymeric materials. This method is broadly tolerant of functional groups and extremely easy to perform. Characteristic properties of resulting poly(triazoles) and preliminary investigations of their adhesive and template recognition properties will be discussed. Among the most important features of the process is that catalytic copper can be recruited from metallic copper surfaces, and that the poly(triazole) products have strong affinity for metal surface.

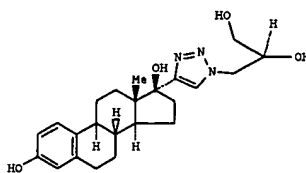
L23 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:227280 CAPLUS
 TI Novel catalysts based on polytriazole dendrimers
 AU Wu, Peng; Feldman, Alina K.; Holzer, Philipp; Fokin, Valery V.; Sharpless, K. Barry
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), ORGN-410 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69FGYM
 DT Conference; Meeting Abstract
 LA English
 AB Based on the recently discovered copper(I)-catalyzed synthesis of 1,2,3-triazoles from azides and terminal alkynes, we have developed an efficient synthesis of a novel class of dendrimers. Our ongoing interest in catalysis and click chemical prompted us to explore metal-binding and catalytic properties of these polytriazole mols. Investigations of the binding behavior of copper in different oxidation states and applications of the resulting complexes to homogeneous catalysis will be described in the presentation.

L23 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:226913 CAPLUS
 TI Copper(I)-catalysis with novel polytriazole ligands
 AU Chan, Timothy R.; Fokin, Valery V.; Sharpless, K. Barry
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), ORGN-041 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69FGYM
 DT Conference; Meeting Abstract
 LA English
 AB The recently discovered copper(I)-catalyzed reaction between azides and terminal alkynes leading to 1,4-disubstituted [1,2,3]-triazoles exhibits high efficiency with a remarkably broad scope. Performing equally well in a variety of solvents and conditions, it has already enabled a multitude of applications in biol., chemical, and materials science. To further improve the efficiency and user-friendliness of the process, we have developed polytriazole ligands which activate copper(I) while simultaneously protecting it from undesired oxidns. and degradation pathways. These polytriazoles belong to a rare class of ligands which are synthesized from the same reaction which they help catalyze. The most potent ligand, TBTA has been successfully applied towards several bioconjugation studies based upon the copper(I)-catalyzed reaction of azides and acetylenes.

L23 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2003:981784 CAPLUS
 DN 140:349802
 TI The growing impact of click chemistry on drug discovery
 AU Kolb, Hartmut C.; Sharpless, K. Barry
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Drug Discovery Today (2003), 8(24), 1128-1137
 CODEN: DDTOP5; ISSN: 1359-6446
 PB Elsevier Science Ltd.
 DT Journal; General Review
 LA English
 AB A review. Click chemical is a modular approach that uses only the most practical and reliable chemical transformations. Its applications are increasingly found in all aspects of drug discovery, ranging from lead finding through combinatorial chemical and target-templated in situ chemical, to proteomics and DNA research, using bioconjugation reactions. The copper(I)-catalyzed 1,2,3-triazole formation from azides and terminal acetylenes is a particularly powerful linking reaction, due to its high degree of dependability, complete specificity, and the bio-compatibility of the reactants. The triazole products are more than just passive linkers; they readily associate with biol. targets, through hydrogen bonding and dipole interactions. Click chemical, a modular approach based on highly reliable chemical transformations, is being applied in all aspects of drug discovery, ranging from lead finding to proteomics and DNA research.
 RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2003:972063 CAPLUS
 DN 140:27830
 TI Process for preparation of 1,4-disubstituted [1,2,3]-triazoles by metal-catalyzed, in particular copper-catalyzed, regioselective Huisgen 1,3-dipolar cycloaddition of azides and acetylenes
 IN Sharpless, K. Barry; Fokin, Valery; Rostovtsev, Vsevolod; Green, Luke; Him, Fahmi
 PA The Scripps Research Institute, USA
 SO PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003101972	A1	20031211	WO 2003-US17311	20030530
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2487424	A1	20031211	CA 2003-2487424	20030530
AU 2003240482	A1	20031219	AU 2003-240482	20030530
EP 1507769	A1	20050223	EP 2003-731490	20030530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671673	A	20050921	CN 2003-817917	20030530
JP 200602099	T	20060119	JP 2004-509665	20030530
US 2005222427	A1	20051006	US 2005-516671	20050516
PRAI US 2002-385041P	P	20020530		
WO 2003-US17311	W	20030530		
OS CASREACT 140:27830				
GI				



AB The invention is directed to a process for Huisgen 1,3-dipolar cycloaddn. of azides and terminal acetylenes for forming 1,4-disubstituted [1,2,3]-triazoles regioselectively, catalyzed by the addition of Cu(II) in the presence of a reducing agent, for reducing

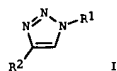
L23 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 AN Cu(II) to Cu(I), in situ, in catalytic amt. The invention also discloses
 TI the use of aq. Cu(I) solns. and other metals such as Au, Ag, Hg, Cd, Pt
 AU and Pd. The advantages include lower reaction temps., even room temp.,
 CS high regioselectivity, use of the cheaper and purer Cu(II) salts, and no
 functional group interference. For instance, I was prepd., in 94% yield,
 by Huisgen 1,3-dipolar cycloaddn. of 17-ethynyl estradiol and
 (S)-3-azidopropane-1,2-diol in the presence of 1 mol% CuSO₄·5H₂O and
 10 mol% sodium ascorbate in water/t-BuOH mixt. at room temp. overnight.
 RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2003:635738 CAPLUS
 TI Copper-catalyzed dipolar cycloadditions
 AU Fokin, Valery V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
 92037, USA
 SO Abstracts of Papers, 226th ACS National Meeting, New York, NY, United
 States, September 7-11, 2003 (2003), ORGN-653 Publisher: American Chemical
 Society, Washington, D. C.
 CODEN: 69EKY9
 DT Conference; Meeting Abstract
 LA English
 AB Azides and alkynes are highly energetic functional
 groups that are easily introduced into organic compds., yet remain inert
 towards the vast majority of functionalities and conditions typical of the
 terrestrial environment. Their copper(I)-catalyzed union to
 give 1,4-triazoles is a remarkably reliable stepwise variant of
 Huisgen's concerted cycloaddn. The process proceeds well in a variety of
 solvents and conditions, ranging from whole serum to organic medium. All
 functional groups studied to date have been tolerated, and different
 copper sources, even copper metal, can be used. Various
 applications enabled by such "bullet-proof" reactivity, from biol. to
 materials science, will be discussed in the presentation.

L23 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2003:135763 CAPLUS
 DN 138:300051
 TI Bioconjugation by copper(I)-catalyzed azide-
 alkyne [3 + 2] cycloaddition
 AU Wang, Qian; Chan, Timothy R.; Hilgraf, Robert; Fokin, Valery V.;
 Sharpless, K. Barry; Finn, M. G.
 CS Departments of Chemistry and Molecular Biology, Scripps Research
 Institute, The Skaggs Institute for Chemical Biology, La Jolla, CA, 92037,
 USA
 SO Journal of the American Chemical Society (2003), 125(11), 3192-3193
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB The copper-catalyzed cycloaddn. reaction between azides
 and alkynes functions efficiently in aqueous solution in the presence
 of a tris(triazolyl)amine ligand. The process has been employed to make
 rapid and reliable covalent connections to micromolar concns. of protein
 decorated with either of the reactive moieties. The chelating ligand
 plays a crucial role in stabilizing the Cu(I) oxidation state and protecting
 the protein from Cu(triazole)-induced denaturation. Because the
 azide and alkyne groups themselves are unreactive with
 protein residues or other biomols., their ligation is of potential utility
 as a general bioconjugation method.
 RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2002:775608 CAPLUS
 TI Copper-catalyzed cycloaddition of azides and
 acetylenes
 AU Rostovtsev, Vsevolod V.; Green, Luke; Sharpless,
 K. Barry; Fokin, V. V.
 CS Department of Chemistry, The Scripps Research Institute, La Jolla, CA,
 92037, USA
 SO Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United
 States, August 18-22, 2002 (2002), ORGN-458 Publisher: American Chemical
 Society, Washington, D. C.
 CODEN: 69CZPZ
 DT Conference; Meeting Abstract
 LA English
 AB Uncatalyzed cycloaddn. of azides and acetylenes
 typically proceeds at elevated temps. and affords a mixture of two
 regioisomers. We have discovered that combination of copper(I)
 iodide (5 mol%) and a base (1equiv.) catalyzes the [2+3] cycloaddn. of
 azides and acetylenes, giving only the 1,4-disubstituted
 1,2,3-triazoles. A wide range of functionality is tolerated.
 The catalyzed reaction proceeds to completion in several hours at room
 temperature, in contrast to the uncatalyzed cycloaddn. The scope and
 mechanism
 of this recently uncovered catalytic process will be presented.

L23 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2002:567200 CAPLUS
 DN 138:39236
 TI A stepwise Huisgen cycloaddition process: copper(I)-catalyzed
 regioselective "ligation" of azides and terminal alkynes
 AU Rostovtsev, Vsevolod V.; Green, Luke G.; Fokin,
 Valery V.; Sharpless, K. Barry
 CS Department of Chemistry and the Skaggs Institute for Chemical Biology, The
 Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Angewandte Chemie, International Edition (2002), 41(14), 2596-2599
 CODEN: ACIEF5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH
 DT Journal
 LA English
 OS CASREACT 138:39236
 GI



AB 1,4-Disubstituted 1,2,3-triazoles I (R1 = PhCH2, PhCH2OCH2,
 1-adamantyl, etc.) R2 = HO2C, Ph, PhOCH2, Et2NCH2, etc.) were readily and
 cleanly prepared via highly efficient and regioselective copper
 (I)-catalyzed cycloaddn. of azides R1N3 with terminal
 alkynes R2C.tpbond.CH in 82-93% yields.
 RE.CMT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his full

(FILE 'HOME' ENTERED AT 10:48:35 ON 21 DEC 2006)

FILE 'CASREACT' ENTERED AT 10:48:46 ON 21 DEC 2006

L1 STRUCTURE UPLOADED
 D
L2 26 SEA SSS SAM L1 (713 REACTIONS)
 D
L3 521 SEA SSS FUL L1 (10377 REACTIONS)
L4 69 SEA ABB=ON PLU=ON L3 AND COPPER
 D
 D BIB ABS
 D BIB ABS HIT

FILE 'CASREACT' ENTERED AT 10:53:48 ON 21 DEC 2006

 D QUE L4 STAT
 D 1-69 BIB ABS FHIT

FILE 'REGISTRY' ENTERED AT 10:57:17 ON 21 DEC 2006

L5 STRUCTURE UPLOADED
 D
L6 0 SEA SSS SAM L5
L7 0 SEA SSS FUL L5
 D QUE L7 STAT
L8 STRUCTURE UPLOADED
 D
L9 0 SEA SSS SAM L8
L10 0 SEA SSS FUL L8
 D QUE L10 STAT

FILE 'REGISTRY' ENTERED AT 11:02:13 ON 21 DEC 2006

L11 STRUCTURE UPLOADED
 D
L12 0 SEA SSS SAM L11
L13 0 SEA SSS FUL L11
 D QUE L11 STAT

FILE 'CAPLUS' ENTERED AT 11:03:04 ON 21 DEC 2006

 E K BARRY SHARPLESS/AU
 E SHARPLESS K BARRY/AU
L14 389 SEA ABB=ON PLU=ON "SHARPLESS K BARRY"/AU
 E FOKIN VALERY/AU
L15 76 SEA ABB=ON PLU=ON ("FOKIN VALERY"/AU OR "FOKIN VALERY V"/AU)

 E ROSTOVTSEV VSEVOLD/AU
L16 17 SEA ABB=ON PLU=ON ("ROSTOVTSEV VSEVOLOD"/AU OR "ROSTOVTSEV
 VSEVOLOD V"/AU OR "ROSTOVTSEV VSEVOLOD VLADIMIROVICH"/AU)
 E GREEN LUKE/AU
L17 17 SEA ABB=ON PLU=ON ("GREEN LUKE"/AU OR "GREEN LUKE G"/AU OR
 "GREEN LUKE GIDEON GRANVILLE"/AU OR "GREEN LUKE M"/AU)
 E HIMO FAHMI/AU
L18 48 SEA ABB=ON PLU=ON "HIMO FAHMI"/AU
L19 489 SEA ABB=ON PLU=ON L14 OR L15 OR L16 OR L17 OR L18
L20 41 SEA ABB=ON PLU=ON L19 AND TRIAZOLE
L21 39 SEA ABB=ON PLU=ON L20 AND AZIDE
L22 36 SEA ABB=ON PLU=ON L21 AND (ACETYLENE OR ALKYNE)

L23

24 SEA ABB=ON PLU=ON L22 AND COPPER
D QUE L23 STAT
D 1-24 BIB ABS

FILE HOME

FILE CASREACT

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 17 Dec 2006 VOL 145 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0

DICTIONARY FILE UPDATES: 20 DEC 2006 HIGHEST RN 916134-56-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE CAPLUS

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Dec 2006 VOL 145 ISS 26
FILE LAST UPDATED: 20 Dec 2006 (20061220/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

100.64

1056.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-18.00

-67.70

STN INTERNATIONAL LOGOFF AT 11:08:05 ON 21 DEC 2006